ARO in Review

U.S. Army Combat Capabilities Development Command (CCDC)
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This report presents an overview of the programs, investment strategies, and accomplishments of the Army Research Office (ARO) for fiscal year 2019 (FY19; 1 Oct. 2018 through 30 Sep. 2019).

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Chapter 01

ARO Mission and Investment Strategy

ARO's mission focuses on driving extramural basic research to ensure the technological superiority of the future Army. This chapter provides an overview of ARO's unique mission, investment strategy, and organizational structure.

This background image is from "Technical Foundation Established for Synthesis of Advanced Coatings and Energetics via Dusty Plasmas" on page 84.

CHAPTER

01 ARO Mission and Investment Strategy

ARO Mission

To fully recognize the value of the ARO mission, one must understand the distinction between basic versus applied research. Basic research is defined by DoD as the "systematic study directed toward greater knowledge or understanding of the fundamental aspects of phenomena and of observable facts without specific applications towards processes or products in mind," while applied research "is a systematic expansion and application of knowledge to develop useful materials, devices, and systems or methods" (DoD 7000.14-R Volume 2B, Chapter 5, 2017).

Basic research drives directed studies toward revolutionary discoveries that will lead (and have led) to groundbreaking new capabilities for the Army in the time frame of thirty years and beyond, whereas applied research focuses on the near-term realization of new or improved technologies to meet a specific need. **Without the long term investment of basic research, the Army will fall behind competitor nations on and off the battlefield.**

The mission of ARO, as part of the U.S. Army Futures Command (AFC) - U.S. Army Combat Capabilities Development Command (CCDC) - Army Research Laboratory (ARL), is to execute the Army's extramural basic research program in the following scientific disciplines: chemical sciences, computing sciences, electronics, life sciences, materials science, mathematical sciences, mechanical sciences, network sciences, and physics.

The goal of this basic research is to drive scientific discoveries that will provide the Army with significant advances in operational capabilities through high-risk, high pay-off research opportunities, primarily with universities, but also with large and small businesses. ARO ensures that this research supports and drives the realization of future research relevant to all of the Army Functional Concepts, the ARL Core Technical Competencies, and the ARL Essential Research Programs (ERPs). The results of these efforts are transitioned to the Army research and development community, industry, or academia for the pursuit of long-term technological advances for the Army.

ARO Investment Strategy

ARO's mission represents the most long-range Army view for new scientific discovery to initiate disruptive new technology, with system applications often 20-30 years away. ARO pursues a long-range investment strategy designed to maintain the Army's overmatch capability in the expanding range of present and future operational capabilities.

ARO competitively selects and funds basic research proposals from educational institutions, nonprofit organizations, and private industry. ARO executes its mission through an aggressive basic science research program on behalf of the Army to create cutting-edge scientific discoveries and to provide and expand the scientific knowledge required to develop and improve weapons systems for land force dominance. The ARO research portfolio consists principally of extramural academic research efforts consisting of single investigator efforts, university-affiliated research centers, and specially tailored outreach programs. Each program has its own objectives and set of advantages as described further in Chapter 2.

ARL's research strategy is organized into the ARL Core Technical Competencies, with current areas of emphasis designated by the ERPs, which aim to address particular technology gaps for the current and future Army. ARO drives fundamental research efforts that will lead to new discoveries and increased understanding of the physical, engineering, and information sciences as they relate to long-term national security needs, in support of all of the ARL Core Technical Competencies and ERPs.

ARO strategy and programs are formulated in concert with the ARL Technical Implementation Plan, the ARL Research Management and Leadership Strategy, the CCDC Centers, and the Army Medical Research and Materiel Command (MRMC). ARO programs and research areas are intimately aligned with, and fully supportive of, the research priorities set within the Department of Defense (DoD), the Army Modernization Priorities, the Army Functional concepts, and the Assistant Secretary of Defense for Research and Engineering [ASD(R&E)] Science and Technology (S&T) Priorities.

ARO serves the following functions in pursuit of its mission:

- Execute an integrated, balanced, and disruptive extramural basic research program
- Create and guide the discovery and application of novel scientific phenomena leading to leap-ahead technologies for the Army
- Drive the application of science to generate new or improved solutions to existing needs
- Accelerate research results transition to applications in all stages of the research and development cycle
- Strengthen the research infrastructures of academic, industrial, and nonprofit laboratories that support the Army
- Focus on research topics that support technologies vital to the Army's future force, combating terrorism and new emerging threats
- Leverage S&T of other defense and government laboratories, academia and industry, and organizations of our allies
- Foster training for scientists and engineers in the scientific disciplines critical to Army needs
- Actively seek creative approaches to enhance the diversity and capabilities of future U.S. research programs by enhancing education and research programs at historically black colleges and universities, and minority-serving institutions

Implementing ARO Strategy

ARO employs multiple programs, initiatives, and investment strategies to fulfill its mission. A snapshot of the ARO research programs is provided in this section, with each program described further in Chapter 2.

Program Snapshot

The research programs managed by ARO range from single investigator research to multidisciplinary/multi-investigator teams. A typical basic research grant within a program may provide funding for a few years, while in other programs, such as research centers affiliated with particular universities, a group of investigators may receive funding for many years to pursue novel research concepts. The programs for the Historically Black Colleges and Universities and Minority Serving Institutions (HBCU/MSI) are aimed at providing infrastructure and incentives to improve the diversity of U.S. basic research programs. In addition to supporting the education of graduate students through basic research grants, the National Defense Science and Engineering Graduate (NDSEG) fellowship program is another mechanism through which ARO fosters the training of a highly-educated workforce skilled in DoD and Army-relevant research, which is critical for the future of the nation. ARO also has extensive programs in outreach to pre-graduate education to encourage and enable the next generation of scientists. In addition, ARO guides the transition of basic research discoveries and advances to the appropriate applied-research and advanced development organizations. ARO is actively engaged in accelerating the transition of discovery into application, in part through involvement in the development of topics and the management of projects in the Small Business Innovation Research (SBIR) and Small Business Technology Transfer (STTR) programs.

Coordination for Program Development and Monitoring

ARO's extramural research programs are formulated in concert with the ARL-wide strategy, including the:

ARL Core Technical Competencies (CTCs)

- Materials and Manufacturing Sciences
- Computational Sciences
- Ballistics Sciences
- Human Sciences
- Propulsion Sciences
- Network and Information Sciences
- Protection Sciences
- Human Autonomy Teaming

ARL Essential Research Programs (ERPs)

- Artificial Intelligence for Maneuver and Mobility
- Foundational Research for Electronic Warfare in Multi-Domain Operations
- Long Range Distributed and Cooperative Engagements
- Convergence of Lethality, Protection and Autonomy to Dominate Ground Combat
- Versatile Tactical Power and Propulsion
- Physics of Soldier Protection to Defeat Evolving Threats
- Science of Additive Manufacturing for Modular Munitions
- Transformational Synthetic Biology for Military Environments
- Quantum Precision Navigation and Timing

ARL Directorates

- Computational and Information Sciences Directorate (ARL CISD)
- Human Research and Engineering Directorate (ARL HRED)
- Sensors and Electron Devices Directorate (ARL SEDD)
- Vehicle Technology Directorate (ARL VTD)
- Weapons and Materials Research Directorate (ARL WMRD)

ARO programs are also formulated through collaborations and consultation with the following DoD and other Federal agencies to ensure complementary investment strategies:

- The CCDC Centers
- CCDC Armaments Center (CCDC AC)
- CCDC Aviation and Missile Center (CCDC AvMC)
- CCDC Army Research Laboratory (CCDC ARL)
- CCDC Chemical Biological Center (CCDC CBC)
- CCDC Command, Control, Computers, Communications, Cyber, Intelligence, Surveillance and Reconnaissance Center (CCDC C5ISR)
- CCDC Data and Analysis Center (CCDC DAC)
- CCDC Ground Vehicle Systems Center (CCDC GVSC)
- CCDC Soldier Center (CCDC SC)
- U.S. Army Medical Research and Materiel Command (MRMC)
- U.S. Army Corps of Engineers (USACE)
- Army Research Institute for the Behavioral and Social Sciences
- U.S. Army Special Operations Command (USASOC)
- U.S. Army Futures and Concepts Center
- Office of Naval Research (ONR)
- Air Force Office of Scientific Research (AFOSR)
- National Institute of Standards and Technology (NIST)
- Defense Advanced Research Projects Agency (DARPA)
- Defense Threat Reduction Agency (DTRA)
- Office of the Secretary of Defense (OSD)
- Intelligence Advanced Research Projects Activity (IARPA)
- National Security Agency (NSA)
- Department of Energy (DoE)
- National Institutes of Health (NIH)
- Environmental Protection Agency (EPA)
- National Science Foundation (NSF)

ARO's extramural research program provides foundational discoveries in support of the ARL Core Competencies and ERPs. While the ARL Directorates and the CCDC Centers are the primary users of the results of the ARO research program, ARO also supports research of interest to USACE, MRMC, other Army Commands, and DoD agencies. The coordination of the ARO extramural program and joint proposal monitoring with other ARL Directorates, CCDC Centers, and other Army laboratories ensures a highly productive and cost-effective Army research effort. The Multidisciplinary University Research Initiative (MURI) teams and University Affiliated Research Centers (UARCs) benefit from the expertise and guidance provided by the ARL Directorates and other DoD, academic, and industry representatives who serve on evaluation panels for each UARC.

The ARO-managed OSD research programs include the University Research Initiative (URI) programs, and the Research and Educational Program (REP) for HBCU/MSIs. These programs fall under the executive oversight of the Defense Basic Research Advisory Group. This group is led by the ASD(R&E) Director for Research, representatives from the ONR, AFOSR, DARPA, ARO, and the Assistant Secretary of the Army (Acquisition, Logistics and Technology) [ASAALT].

ARO programs are also developed and managed with a focus on supporting future Army needs as identified in the Army Modernization Priorities and the Army Functional Concepts. These priorities were published in FY18, with details available at the Army's website (https://www.army.mil/e2/c/downloads/500971.pdf). These priorities emphasize a significant change in how the Army pursues solutions for the current and future warfighter. ARO's strategy is clearly aligned with the needs of the future warfighter and supports all of the Army Modernization Priorities and Army Functional Concepts. As described earlier, ARO's mission represents the most long-range Army view for new scientific discovery to initiate disruptive new technology, with system applications often 20-30 years away. ARO pursues a long-range investment strategy designed to maintain the Army's overmatch capability in the expanding range of present and future operational capabilities.

Review and Evaluation

The ARO Directorates, Divisions, and Programs are evaluated by a wide range of internal (Army) and external (academic, other government) reviews, such as the former biennial ARO Division Reviews and the National Research Council's Technical Assessment Board (TAB) Review. For additional information regarding these review processes, the reader is encouraged to refer to the corresponding presentations and reports from each review (not included here).

ARO Organizational Structure

The organizational structure of ARO mirrors the departmental structure found in many research universities. ARO's scientific divisions are aligned to a specific scientific discipline (e.g., physics), with outreach activities managed through the Technology Integration and Outreach Division, and supported by the Operations Directorate (see Figure 1).

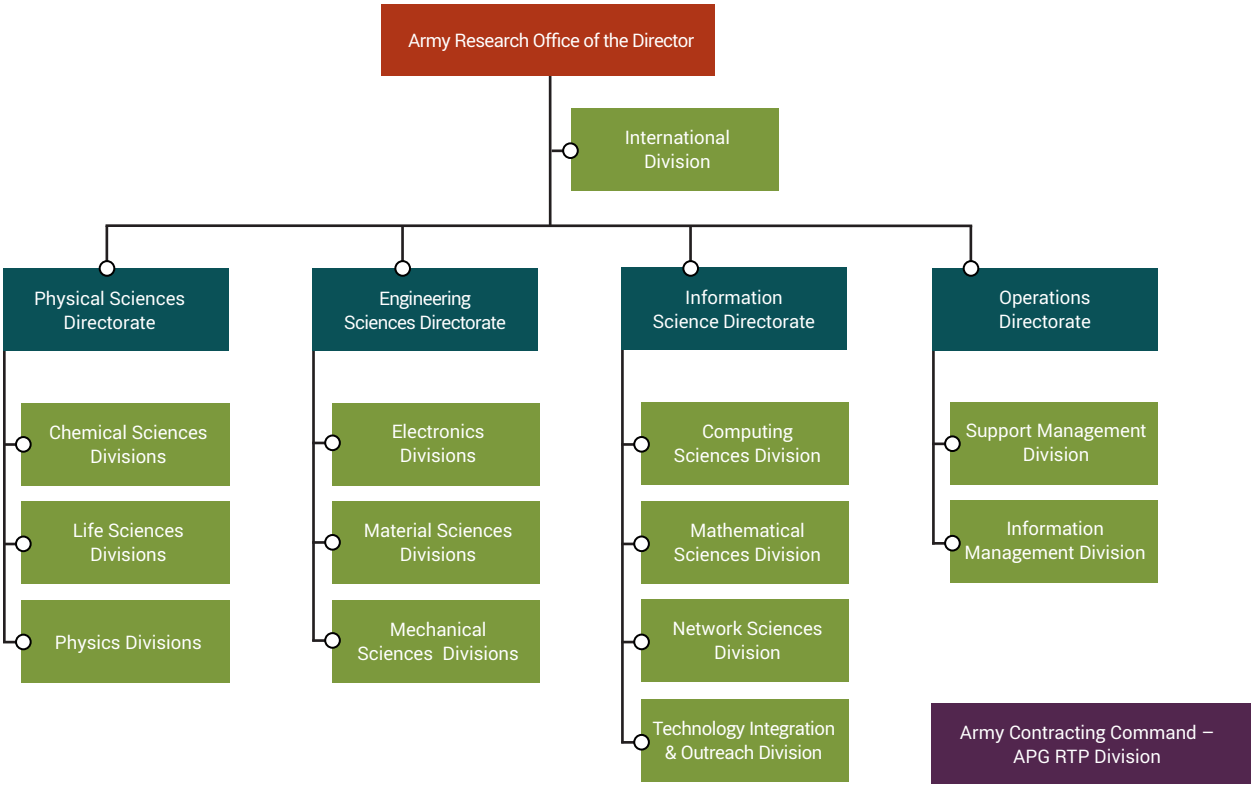

Figure 1. ARO's scientific divisions fall under the Physical Sciences, Engineering Sciences, and Information Sciences Directorates. *Army Contracting Command – Army Proving Ground (APG), Research Triangle Park (RTP) Division is co-located with ARO and executes the contracting needs for ARO funded research. However, it is part of the Army Contracting Command (i.e., not ARL) and also performs contracting activities throughout CCDC.

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Chapter 02

Program Descriptions and Funding Sources

As described in the previous chapter, ARO pursues a variety of investment strategies to meet its mission as the Army's lead extramural basic research agency in chemical sciences, computing sciences, electronics, life sciences, materials science, mathematical sciences, mechanical sciences, network sciences, and physics. ARO, as part of CCDC ARL, is a critical provider of fundamental discoveries in support of all ARL ERPs and Core Technical Competencies. ARO implements its investment strategies through research programs and initiatives that have unique objectives, eligibility requirements, and receives funding from a variety of DoD sources. The visions, objectives, and funding sources of these programs are presented in this chapter.

The selection of research topics, proposal evaluation, and project monitoring are organized within ARO Divisions according to scientific discipline (refer to Chapter 1, Figure 1). Each Division devises a research strategy and develops topics to be included in the ARO Core Broad Agency Announcement (BAA). The ARO Core BAA is provided for reference in Chapter 6. Researchers are encouraged to submit white papers and proposals in areas that support the Division's objectives. The ARO Divisions are not confined to only funding research in the academic departments that align with the Division names; they have the flexibility to find and fund the most promising research to advance their mission regardless of the academic department pursuing a particular research idea.

This background image is from "Imaging The Physical Controls On Rock Debris Surface Properties With A Novel 3D Reconstruction Method" on page 110.

CHAPTER

02 Program Descriptions and Funding Sources

Overview of Program Funding Sources

ARO oversees and participates in the topic generation, proposal solicitation, evaluation, and grant-monitoring activities of programs funded through a variety of DoD agencies, as listed in the following subsections.

Army Funding

The Army funds the majority of the extramural basic research programs managed by ARO, as listed below.

- The ARO Core Research Program, funded through the Army's basic research funds (often referred to as "H57" funds, as described further in the next section).
- The University Research Initiative (URI), which includes these component programs:
  - Multidisciplinary University Research Initiative (MURI) program
  - Presidential Early Career Awards for Scientists and Engineers (PECASE)
  - Defense University Research Instrumentation Program (DURIP)
- Three University Affiliated Research Centers (UARCs)

ARO coordinates with the Office of the Secretary of Defense (OSD) in managing the URI programs and also manages the Army's Small Business Technology Transfer (STTR) program.

Office of the Secretary of Defense (OSD) Funding

The funds for a variety of programs managed or supported by ARO are provided by OSD. These include:

- Research and Educational Program (REP) for Historically Black Colleges and Universities and Minority Serving Institutions (HBCU/MSI)
- National Defense Science and Engineering Graduate (NDSEG) Fellowships
- Educational Outreach Activities

These activities are mandated by DoD's Chief Technology Office, the Office of the Assistant Secretary of Defense for Research and Engineering [OASD(R&E)]. Each of these OSD-funded programs has a unique focus and/or a unique target audience. ARO has been designated by OASD(R&E) as the lead agency for the implementation of REP for HBCU/MSI activities on behalf of the three Services. OSD oversees ARO management of the Army-funded URI and its component programs (MURI, PECASE, and DURIP).

Other Funding Sources

In addition to the Army- and OSD-funded programs described earlier in this section, ARO leverages funds from other DoD sources (e.g., DARPA) to support a variety of external programs with specific research focuses. These joint programs have objectives consistent with the strategies of the corresponding ARO Program. Due to the unique nature of these cooperative efforts, each externally-funded effort is discussed within the chapter of the aligned scientific Division.

ARO Core (H57) Research Program

ARO Core Research Program activities fall under five categories, discussed in the following subsections:

(a) Single Investigator awards;

(b) Short Term Innovative Research efforts;

(c) Young Investigator Program;

(d) support for conferences, workshops, and symposia;

(e) international programs; and

(f) special programs. A summary of the Core Research Program budget is presented in Table 5.

ARO's mission is focused on the development and execution of the majority of the Army's extramural basic research program. As described in Chapter 1, one must understand the distinction of basic vs applied research to fully recognize the value of the ARO mission. ARO's Core (H57) Research Program represents the primary or "core" mechanism ARO uses to create and execute long-term basic research that will (and has) led to new capabilities for the future Army.

ARO's Core (H57) Research Program is a subset of Army 6.1 research. The nomenclature "6.1" is a shorthand reference to basic research, as described in the annual DoD budget documents submitted to request appropriations from Congress (refer to DoD 7000.14-R, Volume 2B, Chapter 5). For comparison, "6.2" refers to applied research and "6.3" is for advanced technology development. The term "H57" refers to the portion of the Army's budget specifically associated with extramural basic research, which are activities that are performed at external institutions versus studies performed at in-house (intramural) Army laboratories.

Within the ARO Core Program and its ongoing BAA, research proposals are sought from educational institutions, nonprofit organizations, and commercial organizations for basic research in electronics, physics, and the chemical, computing, life, materials, mathematical, mechanical, and network sciences.

The goal of this program is to utilize world-class and worldwide academic expertise to discover and exploit novel scientific discoveries, primarily at universities, to provide the current and future force with critical new or enhanced capabilities.

Single Investigator (SI) Program

The goal of the SI program is to pursue the most innovative, high-risk, and high-payoff ideas in basic research. Research proposals within the SI Program are received throughout the year in a continuously-open, worldwide BAA solicitation. This program focuses on basic research efforts by one or two faculty members along with supporting graduate students and/or postdoctoral researchers and is typically a three-year grant. This program, as for all program elements that fall under the overarching ARO Core Program, enables the Army to invest and drive national academic research toward areas of interest to the future Army. As the grants are on a three-year cycle, approximately one third of the extramural portfolio can be reinvested into new or advancing areas each year. This program provides the Army with a dynamic method for rapidly investing or divesting in research to ensure the realization of foundational discoveries that will enable future Army capabilities.

Short Term Innovative Research (STIR) Program

The objective of the STIR Program is to explore high-risk initial proof-of-concept ideas within a nine-month time frame. Research proposals are sought from educational institutions, nonprofit organizations, or private industry. If a STIR effort's results are promising, the investigator may be encouraged to submit a proposal to be evaluated for potential longer-term funding options, such as an SI award.

Young Investigator Program (YIP)

The objective of the YIP is to attract outstanding young university faculty to Army-relevant research questions, to support their research, and to encourage their teaching and research careers. Outstanding YIP projects may be considered for the prestigious PECASE award.

Conferences, Workshops, and Symposia Support Program

The ARO Core Program also provides funding for organizing and facilitating scientific and technical conferences, workshops, and symposia. This program provides a method for conducting scientific and technical meetings that facilitate the exchange of scientific information relevant to the long-term basic research interests of the Army and help define research needs, thrusts, opportunities, and innovation. In particular, workshops are a key mechanism ARO uses to identify new research areas with the greatest opportunities for scientific breakthroughs that will revolutionize future Army capabilities.

International Programs

Beginning in FY16, ARO initiated international programs with the goal of identifying academic investigators who are the forerunners in particular fields of research of which U.S. scientists do not currently hold the lead. Based on a detailed data analytics study that assessed 39 countries and their research publication output from 2009-2014, ARO identified scientific areas critical to the future Army, components of which are led by researchers outside of the U.S. These areas were grouped into three key geographic locations: the Atlantic, Pacific, and Americas regions.

These international programs are part of ARL and ARO's comprehensive approach to ensure that Army basic research funds are used efficiently to find the scientists best suited to drive high-risk, high-payoff Army crucial research, regardless of whether these researchers are in the U.S. or abroad. The ARO International Program Managers (PMs) are each aligned to an ARO Division and focus on key research areas to identify international investigators with skills and ideas in areas not led by researchers within the U.S., as well as to engage and partner those researchers with existing Army and DoD programs. These international research areas, the corresponding aligned Division, and the locations where the International PMs are stationed are listed below:

- Energy Transport and Storage (Chemical Sciences Division) - Tokyo, Japan
- Synthetic Biology (Life Sciences Division) - Tokyo, Japan
- Human Dimension (Life Sciences Division) - London, United Kingdom
- Innovation in Materials (Materials Science Division) - London, United Kingdom (vacant in FY19)
- Network Science and Intelligent Systems (Network Sciences Division) - London, United Kingdom
- Quantum Scale Materials (Physics Division) - Tokyo, Japan

Special Programs

Although the programs listed earlier in this section constitute the primary use of H57 funds, the ARO Core Research Program also supports a variety of special programs. The Research Instrumentation (RI) Program is designed to improve the capabilities of U.S. institutions of higher education to conduct research and educate scientists and engineers in areas important to national defense, and funds may be provided to purchase instrumentation in support of this research or in the development of new research capabilities. However, the majority of instrumentation support awarded through ARO is provided through the Defense University Research Instrumentation Program (DURIP). The ARO Core Research Program also co-funds awards selected through the Army's High School Apprenticeship Program (HSAP) and Undergraduate Research Apprenticeship Program (URAP), which is managed through ARO's Technology Integration and Outreach Division's Educational Outreach Activities.

Multidisciplinary University Research Initiative (MURI)

The MURI Program is part of the University Research Initiative (URI) and supports research teams whose research efforts intersect more than one traditional discipline. A multidisciplinary effort can accelerate research progress in areas particularly suited to this approach by cross-fertilization of ideas, can hasten the transition of basic research findings to practical applications, and can help to train students in science and/or engineering in areas of importance to DoD. In contrast with ARO Core program SI research projects, MURI projects support centers whose efforts require a large and highly collaborative multidisciplinary research effort. These are typically funded at $1.25 million per year for three years with an option for two additional years. The efforts are expected to enable more rapid research and development breakthroughs and to promote eventual transition to Army applications.

Oversight of the MURI program comes from the Basic Research Office of OASD(R&E) to the Service Research Offices (OXRs), where OXR PMs manage the MURI projects. The OXRs include ARO, the Air Force Office of Scientific Research (AFOSR), and the Office of Naval Research (ONR). OXR PMs have significant flexibility and discretion in how the individual projects are monitored and managed, while OASD(R&E) defends the program to higher levels in OSD and has responsibility for overall direction and oversight. Selection of Army research topics and the eventual awards are reviewed and approved by OASD(R&E) under a formal acquisition process.

The full list of all ARO-managed MURI projects that were active in FY19 are described in Chapter 5.

Eight MURI projects were selected for funding and began in FY19. These projects are based on proposals submitted to the FY19 MURI FOA, which was released in late FY18. Each new start project, lead investigator, and lead performing organization are listed here, immediately below the corresponding MURI topic, topic authors/PMs, and the ARO Division responsible for monitoring the project.

The following eight proposals were selected to be the FY19 new starts for the MURI Program:

Topic: Clearing Your Head: The Glymphatic System and Restorative Effects of Sleep
PMs: **Dr. Matthew Munson (Mechanical Sciences) and Dr. Frederick Gregory (Life Sciences)**
Project Selected: *How sleep clears your brain: Slow waves, glymphatic waste removal, and synaptic down-selection*
Lead PI: **Dr. Maiken Nedergaard, University of Rochester**

Topic: Foundations of Emergent Computation and Self-Organized Adaptation
PMs: **Dr. Samuel Stanton (Mechanical Sciences) and Dr. Paul Baker (Physics)**
Project Selected: *Formal Foundations of Algorithmic Matter and Emergent Computation*
Lead PI: **Dr. Dana Randall, Georgia Institute of Technology**

Topic: Multi-layer Network Modeling of Plant and Pollen Distribution across Space and Time
PMs: **Dr. Micheline Strand (Life Sciences) and Dr. Lisa Troyer (Life Sciences)**
Project Selected: *Networked palynology models of pollen and human systems*
Lead PI: **Dr. Anthony Grubesic, Arizona State University**

Topic: Near Field Radiative Heat Energy Transfer between Nanostructured Materials
PMs: **Dr. Pani Varanasi (Materials Science) and Dr. Marc Ulrich (Physics)**
Project Selected: *Near-Field Radiative Heat Transfer and Energy Conversion in Nanogaps of Nano- and Meta-Structured Materials*
Lead PI: **Dr. Pramod Sangi Reddy, University of Michigan - Ann Arbor**

Topic: Networked Interactions Governing Community Dynamics
PMs: **Dr. Robert Kokoska (Life Sciences) and Dr. Derya Cansever (Network Science)**
Project Selected: *Investigating energy efficiency, information processing and control architectures of microbial community interaction networks*
Lead PI: **Dr. James Boedicker, University of Southern California**

Topic: Prediction and Control in Particulate Systems
PMs: **Dr. Joseph Myers (Mathematical Sciences) and Dr. Julia Barzyk (Mechanical Sciences)**
Project Selected: *Predicting and Controlling the Response of Particulate Systems through Grain-Scale Engineering*
Lead PI: **Dr. Jose Andrade, California Institute of Technology**

Topic: Reactive and non-Reactive Scattering from Targeted Molecular Quantum States
PMs: **Dr. James Parker (Chemical Sciences) and Dr. Paul Baker (Physics)**
Project Selected: *Quantum State Control of Molecular Collision Dynamics*
Lead PI: **Dr. Arthur Suits, University of Missouri**

Topic: Unified Decision Theory: From Bounded to Unbounded Rationality
PMs: **Dr. Purush Iyer (Network Science) and Dr. Edward Palazzolo (Network Science)**
Project Selected: *Foundations of Decision Making with Behavioral and Computational Constraints*
Lead PI: **Dr. Ali Jadbabaie-Moghadam, Massachusetts Institute of Technology**

The following eight topics were published in FY19 and constitute the ARO portion of the FY20 MURI BAA:

Topic: Adaptive and Adversarial Machine Learning
PM: **Dr. Purush Iyer (Network Science)**

Topic: Axion Electrodynamics beyond Maxwell's Equations
PMs: **Dr. Joe Qui, (Electronics) and Dr. Marc Ulrich (Physics)**

Topic: Engineering Endosymbionts to Produce Novel Functional Materials
PMs: Dr. Micheline Strand (Life Sciences) and Dr. Pani Varanasi (Materials Science)

Topic: Information Exchange Network Dynamics
PM: **Dr. Derya Cansever (Network Science) and Dr. Edward Palazzolo (Network Science)**

Topic: Mathematical Intelligence: Machines with More Fundamental Capabilities
PMs: **Dr. Joe Myers (Mathematical Sciences) and Dr. Sara Gamble (Physics)**

Topic: Quantum State Engineering for Enhanced Metrology
PMs: **Dr. Paul Baker (Physics) and Dr. Joe Qui, (Electronics)**

Topic: Solution Electrochemistry without Electrodes
PM: **Dr. Robert Mantz (Chemical Sciences)**

Topic: Stimuli-Responsive Mechanical Metamaterials
PMs: **Dr. Samuel Stanton (Mechanical Sciences) and Dr. Dawanne Poree (Chemical Sciences)**

Presidential Early Career Award for Scientists and Engineers (PECASE)

The PECASE program, also part of the URI program, attracts outstanding young university faculty members, supporting their research, and encouraging their teaching and research careers. PECASE awards are the highest honor bestowed by the Army to extramural scientists and engineers beginning their independent research careers. Each award averages $200K/year for five years. PECASE awards are based in part on two important criteria: 1) innovative research at the frontiers of science and technology that is relevant to the mission of the sponsoring agency, and 2) community service demonstrated through scientific leadership, education, and outreach. The PECASE winners for each calendar year's competition are typically announced by the White House.

The 2015, 2016, and 2017 PECASE awardees were announced by the White House and funded as new-start projects in FY19. The 2018 PECASE nominees are awaiting White House approval to officially begin as PECASE candidates. The 2018 PECASE nominees were funded in FY19 as Army Early Career Award for Scientists and Engineers (ECASE) new-start projects.

2015 PECASE Awardees (awarded in FY19)

- Dhruv Batra, Virginia Polytechnic Institute & State University, Purush Iyer (Network Science)
- Joseph Checkelsky, Massachusetts Institute of Technology, Marc Ulrich (Physics)
- Phillip Christopher, University of California, Riverside, Robert Mantz (Chemical Sciences)
- Jinglin Fu, Rutgers University-Camden, Stephanie McElhinny (Biological Sciences)

2016 PECASE Awardees (awarded in FY19)

- Gordon Wetzstein, Stanford University, Hamid Krim (Computing Sciences)
- Jenny Suckale, Stanford University, Julia Barzyk (Mechanical Sciences)
- Percy Liang, Stanford University, Purush Iyer (Network Science)
- Yuji Zhao, Arizona State University, Michael Gerhold (Electronics)

2017 PECASE Awardees (awarded in FY19)

- Steven Brunton, University of Washington, Matthew Munson (Mechanical Sciences)
- Jeff Thompson, Princeton University, Sara Gamble (Physics)
- Domenic Forte, University of Florida, Cliff Wang (Computing Sciences)
- Katharine Tibbetts, Virginia Commonwealth University, James Parker (Chemical Sciences)

2018 ECASE Awardees

- Bo Zhen, University of Pennsylvania, Michael Gerhold (Electronics)
- Lauren Zarzar, Pennsylvania State University, Dawanne Poree (Chemical Sciences)
- Ehsan Hoque, University of Rochester, Edward Palazzolo (Network Science)
- Jerome Fox, University of Colorado-Boulder, Stephanie McElhinny (Life Sciences)

Defense University Research Instrumentation Program (DURIP)

DURIP, also part of the URI program, supports the purchase of state-of-the-art equipment that augments current university capabilities or develops new capabilities to perform cutting edge defense research. DURIP meets a critical need by enabling university researchers to purchase equipment costing $50K or more to conduct DoD-relevant research. In FY19, the Army awarded 50 grants at $9.9M total, with an average award of $350K.

University Affiliated Research Centers (UARCS)

The Army's University Affiliated Research Centers (UARCs) are strategic DoD-established research organizations at universities. The UARCs were formally established in May 1996 by OASD(R&E) to advance DoD long-term goals by pursuing leading-edge basic research and to maintain core competencies in specific domains unique to each UARC, for the benefit of DoD. One DoD Agency is formally designated by OASD(R&E) to be the primary sponsor for each UARC. The primary sponsor ensures DoD UARC management policies and procedures are properly implemented. Collaborations among UARCs and the educational and research resources available at the associated universities can enhance each UARC's ability to meet the long-term goals of DoD.

ARO is the primary sponsor for two UARCs and co-manages a third.

- The Army's Institute for Soldier Nanotechnologies (ISN), located at the Massachusetts Institute of Technology (MIT).
- The Army's Institute for Collaborative Biotechnologies (ICB), located at the University of California - Santa Barbara, with academic partners at MIT and the California Institute of Technology.
- The Army's Institute for Creative Technologies (ICT), located at the University of Southern California. In contrast to the ISN and ICB, the ICT is co-managed between ARO and the CCDC Soldier Center (SC), where ARO is responsible for 6.1 efforts, and CCDC SC is responsible for managing the 6.2 and 6.3 efforts.

Minerva Research Initiative (MRI)

The Minerva Research Initiative (MRI) is a DoD-sponsored, university-based social science basic research program initiated by the Secretary of Defense and focuses on areas of strategic importance to U.S. national security policy. It seeks to increase the intellectual capital in the social and behavioral sciences and improve DoD's ability to address future challenges and build bridges between DoD and the social and behavioral sciences community, with a focus on the National Defense Strategy and basic research missions of the tri-service branches (U.S. Army, U.S. Air Force, U.S. Navy). Minerva brings together universities, research institutions, and individual scholars and supports multidisciplinary and cross-institutional projects addressing specific topic areas determined by DoD.

Minerva projects are funded up to a five-year base period, with awards ranging from small, single investigator grants for two to three years to large multidisciplinary projects for $1-2 million per year for five years. The program is overseen by the U.S. Air Force and U.S. Navy and OSD; with currently managing projects (2-5 year duration) dealing with models of multi-state burden-sharing to mitigate conflict and establish sociopolitical stability

in fragile states, assessment of post-conflict crises and factors impacting social order; and development of new models to predict causes and consequences of sociopolitical stability and rise of violent extremist organizations. ARO also provides scientific, technical, and managerial support to OSD in managing projects in these areas.

The titles of ARO-managed FY19 new-start Minerva projects are listed below, followed by the name of the lead PI, the performing organization, and the award duration.

- *A Network Analytic Study of the Determinants and Consequences of Burden Sharing in International Alliances and Defense Cooperation Agreements,* 1945-2015, PI: Professor Zeev Maoz, University of California-Davis, FY19-FY22.
- *Rising to the Top: Armed Group Consolidation in Civil Wars and Fragile States,* PI: Professor Michael Gabbay, University of Washington, FY19-FY22.
- *Integrating Structural Theories of Revolution with Evolutionary Models to Predict Societal Resilience,* Professor Sergey Gavrilets, University of Tennessee - Knoxville, FY18-FY21
- *Informal Economies, Societal Stability, and Regime Resilience in China and Russia,* Professor Marina Zaloznaya, University of Iowa, FY18-FY21

Small Business Innovation Research (SBIR) And Small Business Technology Transfer (STTR) Programs

Congress established the SBIR and STTR programs in 1982 and 1992, respectively, to provide small businesses and research institutions with opportunities to participate in government sponsored R&D. The DoD SBIR and STTR programs are overseen by the Office of the Under Secretary of Defense for Research and Engineering. The Army-wide SBIR Program is managed at Headquarters, CCDC, while the Army-wide STTR Program is managed by CCDC ARL at ARO. In contrast to the basic research programs managed by ARO, the SBIR and STTR programs focus primarily on feasibility studies leading to prototype demonstration of technology for specific applications.

Purpose and Mission

The purpose of the SBIR and STTR programs is to: 1) stimulate technological innovation; 2) use small business to meet Federal R&D needs; 3) foster and encourage participation by socially and economically disadvantaged small business concerns (SBCs), in technological innovation; and 4) increase private sector commercialization of innovations derived from Federal R&D, thereby increasing competition, productivity, and economic growth. The STTR program has the additional requirement that small companies must partner with universities, federally funded research and development centers, or other non-profit research institutions to work collaboratively to develop and transition ideas from the laboratory to the marketplace.

Three-Phase Process

The SBIR and STTR programs use a three-phase process, reflecting the high degree of technical risk involved in funding research, and developing and commercializing cutting edge technologies. The basic parameters of this three-phase process for both programs within the Army are shown in Table 1.

Phase I. Phase I of the SBIR and STTR programs involves a feasibility study that determines the scientific, technical, and commercial merit and feasibility of a concept. Each SBIR and STTR BAA contains topics seeking specific solutions to stated government needs. Phase I proposals must respond to a specific topic in the BAA, and proposals are competitively judged on the basis of scientific, technical, and commercial merit. The Phase I evaluation and award process marks the entry point to the program and cannot be bypassed.

Phase II. Phase II represents a major research and development effort, culminating in a well-defined deliverable prototype (i.e., a technology, product, or service). The Phase II selection process is also competitive. Phase I contractors can submit Phase II proposals during one of the respective program's submissions cycles, as there are no separate Phase II BAAs. Typically 50% of Phase II proposals are selected for award. SBIR Phase II awardees may be selected to receive additional funds as an invited Subsequent Phase II, Phase II Enhancement, or via the Commercialization Readiness Program (CRP). STTR Phase II awards may also be selected to receive additional funds as an invited Sequential Phase II.

Phase III. In Phase III, the small business or research institute is expected to obtain funding from the private sector and/or non-SBIR/STTR government sources to develop products, production, services, R&D, or any combination thereof into a viable product or service for sale in military or private sector markets. Commercialization is the ultimate goal of the SBIR and STTR programs.

Table 1

Three-phase process of the SBIR and STTR programs. Phase I is an assessment of technical merit and feasibility, Phase II is a larger R&D effort often resulting in a deliverable prototype, and Phase III is a project derived from, extending, or logically concluding prior SBIR/STTR work, generally to develop a viable product or service for military or commercial markets.

	SBIR Contract Limits	STTR Contract Limits
Phase I	• 6 months, $100K max • 3-month option (at Government's discretion), $50K max, to fund interim Phase II efforts	• 6 months, $150K max • No options
Phase II	• 2 years, $1 million max	• 2 years, $1 million max
Subsequent Phase II	• 2 years, $1 million max	• 2 years, $1 million max
Phase II Enhancement	• 2 years, $500K matching funds max	• n/a
Phase III	• No time or size limit • No SBIR/STTR set-aside funds	• No time or size limit • No SBIR/STTR set-aside funds

Army FY19 STTR Program

ARO manages the Army-wide STTR program and has since the program's inception in 1992. ARO coordinates participation of nine (9) Army components and commands and invests in all Army Modernization priorities. In FY19, the budget was $37.4 million, up 7% from FY18 when it was $35 million. Participating components include: CCDC AvMC, CCDC AC, CCDC ARL ARO, CCDC C5ISR, CCDC CBC, CCDC SC, CCDC GVSC, Corp of Engineers (CoE)-ERDC and MRDC.

Army STTR teamed with U.S. Army Special Operations Command (USASOC) to pilot a rapid-response, prototyping-transition program, bringing innovative technologies direct to the warfighter. This ARO USASOC partnership involves all phases of R&D life cycle processes: requirement definition, vendor selection, prototype

delivery, and follow-on testing and procurement/sustainment. On 10 September 2019 ARO USASOC co-hosted an Industry Day, allowing small businesses and universities from across the nation to learn more about these USASOC warfighting special topics, as well as provide a forum for better teaming partnerships among the Industry Day participants, with stronger proposals and more innovative ideas/solutions for warfighter vetting. This pilot program will invest ~$10M in STTR Phase 1 and Phase 2 pilot projects and compress the Army STTR life cycle from 6-years to 2-years, a 67% schedule reduction; resulting in rapid prototyping and fielding during the course of 2019-2020.

An Army STTR small business/university team of Boston Fusion Corporation, Arizona State University and Sharper Insight Corporation received Army STTR Phase 1 and Phase 2 investments to develop Big Open-Source Social Science (BOSSS). BOSSS provides the U.S. military with rapid and reliable situational awareness (SA) of the human landscape – the social structures, beliefs, values, persons of influence, behaviors, economy, military, politics, and other 'hot topics' – for their area of operation. BOSSS structures and organizes data by applying state-of-the-art search, natural language processing, and data association techniques to rapidly search, retrieve, process and transform data into frameworks for social understanding, grounded in well-founded social science theory. The Army Corps of Engineers awarded an initial $88K STTR Phase 3 to Boston Fusion to integrate the BOSSS platform across the Army and DoD. BOSSS vastly improves existing extraction, processing and modeling of key groups, events, issues and concerns. BOSSS improves operational design and planning, support analysis of civil considerations and open sources and yields missions that more thoroughly consider key issues of integrated campaigning and the information environment.

ARO FY19 SBIR and STTR Topics

The following SBIR and Chemical-Biological Defense (CBD) SBIR topics were published in an FY19 SBIR BAA. The lead topic author (who serves as the topic PM) and corresponding Division are listed with each topic.

- *Non-Line of Sight Directional Control Technology;* Dr. Stephen Lee, ARO
- R*obust Wideband Full Duplex Radios;* Dr. Robert Ulman, Network Sciences
- *New Concept for a Low Distortion, High-Power, High-Efficiency mm-Wave RF Power Amplifier Circuit;* Dr. James Harvey, Electronics
- *Solid Oxide Fuel Cell (SOFC) Power System;* Dr. Robert Mantz, Chemical Sciences
- *Ultra-narrow linewidth, high power semiconductor laser;* Dr. Michael Gerhold, Electronics
- *Cleaning Personal Protective Equipment of Military Firefighters;* Dr. Dawanne Poree, Chemical Sciences
- *Military Working Dog Decontamination Kit;* Dr. Dawanne Poree, Chemical Sciences
- *On-site Treatment of Contaminated Equipment;* Dr. Dawanne Poree, Chemical Sciences

The following SBIR and Chemical-Biological Defense (CBD) SBIR topics were published in an FY19 SBIR BAA. The lead topic author (who serves as the topic PM) and corresponding Division are listed with each topic.

- *Uniform Dispersion and Alignment of Short Fiber Composite Reinforcement* ; Dr. Michael Bakas, Materials Science
- *Diamond Electron Amplifiers;* Dr. Joe Qiu, Electronics
- *High-Speed Mid-Infrared Free-Space Laser Communications;* Dr. Michael Gerhold, Electronics
- *Isogeometric Analysis Methods for High Fidelity Mobility Applications;* Dr. Joe Myers, Mathematical Sciences
- *Low Temperature Deposition of Magnetic Materials on Topological Materials;* Dr. Marc Ulrich, Physics
- *Exploiting Single Nucleotide Polymorphisms for Extreme Performance;* Dr. Micheline Strand, Life Sciences

- *Intrinsically Interference And Jamming-Resistant High Frequency (HF) Radios;* Dr. Joe Qiu, Electronics
- *Millimeter Waveforms For Tactical Networking;* Dr. Dereya Cansever, Network Sciences
- *Position, Navigation and Timing (PNT) Without The Global Positioning System (GPS);* Dr. Dereya Cansever, Network Sciences
- *Tactical Edge Sensor Processing;* Dr. Dereya Cansever, Network Sciences
- *Adaptable Tactical Communications;* Dr. Dereya Cansever, Network Sciences
- *Phased-Array Antennas For Advanced Extremely High Frequency Satellite Communications;* Dr. Joe Qiu, Electronics
- *Standoff Electronic Denial;* Dr. Michael Gerhold, Electronics

ARO FY19 SBIR and STTR Phase II Contract Awards

The following SBIR,Chemical-Biological Defense (CBD) SBIR topics were selected for Phase II contracts in FY19. The lead topic author/PM and corresponding Division are listed following each topic title.

- *Universal Software-Defined Receiver for Assured Positioning, Navigation, and Timing (PNT)*; Dr. Joe Qiu, Electronics
- *Reproducible high yield production of structural proteins for biologically-derived fibers as an alternative to nylon;* Dr. Stephanie McElhinny, Life Sciences
- *High-Speed Cryogenic Optical Connector for Focal Plane Array Read-out;* Dr. Michael Gerhold, Electronics
- *THz Superradiant Emitters Based on Quantum Dots in GaAs Driven at 1550 nm;* Dr. Joe Qiu, Electronics
- *Transforming 3D Reconnaissance Data into Geospatial Intelligence;* Dr. Michael Coyle, Computing Sciences

ARO FY19 SBIR and CBD SBIR Subsequent Phase II Contract Awards

The following SBIR and CBD SBIR topics were selected for a Subsequent Phase II contract in FY19. The lead topic author/PM and corresponding Division are listed following the topic title.

- *Nanostructured Electrode Materials for Enhanced Biological Charge Transfer;* Dr. Stephanie McElhinny, Chemical Sciences
- *Development of comprehensive biothreat identifier - Zeteo Threat Agent Detection System (zTADS);* Dr. Dawanne Poree, Chemical Sciences
- *A Next Generation, High-Precision, Field Drug Detection System; Dawanne Poree,* Dr. Chemical Sciences
- *Detection of "active" biological toxins by exploiting native binding specificities;* Dr. Dawanne Poree, Chemical Sciences
- *In Situ Production of Biocidal Reactive Oxygen via Directed Energy;* Dr. Stephen Lee, ARO

ARO FY19 STTR and CBD STTR Subsequent Phase II Contract Awards

The following STTR topics were selected for Subsequent Phase II contracts in FY19. The lead topic author/PM and corresponding Division are listed following each topic title.

- *Stochastic Electromagnetic / Circuit Analysis;* Dr. James Harvey, Electronics
- *Scalable Manufacturing of Functional Yarns for Textile Energy Storage;* Dr. Robert Mantz, Chemical Sciences
- *Parallel Two-Electron Reduced Density Matrix Based Electronic Structure Software for Highly Correlated Molecules and Materials;* Dr. James Parker, Chemical Sciences
- *Pulse Voltammetry Tools for Accurate and Rapid Analysis of Batteries;* Dr. Robert Mantz, Chemical Sciences
- *High-Performance Activewear and Workwear made from Virgin and Recycled Cotton;* Dr. Robert Mantz, Chemical Sciences
- *Tools for Parallel Adaptive Simulation of Multiphase Ballistic Flows;* Dr. Joseph Myers, Mathematical Sciences
- *ADA Conformable Wearable Battery-Hybrid Electrical Energy Storage System: A Rechargeable, Safe and High Performance Energy Storage Solution;* Dr. Robert Mantz, Chemical Sciences

ARO FY19 SBIR and CBD SBIR Phase III Contract Awards

The following SBIR and CBD SBIR topics were awarded a Phase III contract in FY19. The lead topic author/PM and corresponding Division are listed following each topic title. Phase III revenues can be obtained from Government or private customers, but cannot be SBIR/STTR funds.

- *Advancement of Capabilities, Products, and Sensors in Chem/Bio Detection, Quantification, and Mitigation IDIQ*; Dr. Stephen Lee, ARO

ARO FY19 STTR Phase III Contract Awards

The following STTR topics were awarded a Phase III contract in FY19. The lead topic author/PM and corresponding Division are listed following the topic title. Phase III revenues can be obtained from Government or private customers, but cannot be SBIR/STTR funds.

- *ID/IQ for USASOC Engineering Analysis and Support;* Dr. Stephen Lee, Chemical Sciences
- *Artificial Intelligence (AI) for Tactical Power, Operations and Advanced Manufacturing;* Dr. Stephen Lee, ARO
- *Rapid Detection and Identification of Biological Events;* Dr. Dawanne Poree, Chemical Sciences

Contract Evaluation and Funding

The Army receives Phase I and Phase II proposals in response to SBIR, STTR, CBD-SBIR/STTR and OSD-SBIR/STTR topics that are published during solicitation periods throughout each fiscal year. Proposals are evaluated against published evaluation criteria and selected for contract award. Contract awards are made pending completion of successful negotiations with the small businesses and availability of funds.

Historically Black Colleges and Universities And Minority-Serving Institutions (HBCU/MSI) Programs

The programs for HBCU/MSIs are a significant part of the ARO portfolio. These programs are discussed in the following subsections.

ARO (Core) HBCU/MSI Program

Academic institutions classified as HBCU/MSIs may submit proposals to the ARO Core BAA, as for any other institution, and are evaluated and selected according to the same evaluation criteria and process established for all proposal submissions to the Core BAA. In FY19, ARO supported 111 agreements with HBCU/MSIs receiving over $8.4 million in FY19 core funding, including 45 new starts listed here.

The new-start HBCU/MSI research grants are listed below, with the project title followed by the PI, performing organization, ARO PM, and corresponding scientific division.

- *Supersymmetry in Optics: Beyond Traditional Supersymmetric Quantum Mechanics,* Professor Arash Mafi, University of New Mexico – Albuquerque; Dr. Richard Hammond, Physics Division
- *Fast Chemical Transformations in Energetic Materials Under Conditions of High Pressure, Temperature and Strain Rate,* Professor Mohammad Mahmood, Howard University; Dr. James Parker, Chemical Sciences Division
- *Analysis and Control of Phase-Amplitude Cluster Synchronization in Structural Brain Networks,* Professor Fabio Pasqualetti, University of California – Riverside; Dr. Derya Cansever, Network Sciences Division
- *Multi-color filaments for extended range, applied to remote sensing and laser induced EMP,* Professor Jean-Claude Diels, University of New Mexico – Albuquerque; Dr. Richard Hammond, Physics Division
- *Multiblock Copolymers with Sulfonated Poly (arylene ethers) and Fluoropolymers for Improved Protective Capabilities and Energy Efficient Devices,* Professor David Suleiman, University of Puerto Rico – Mayaguez; Dr. Dawanne Poree, Chemical Sciences Division
- *Sparsity-based Design for Robust Deep Learning - Topic C. iii (3),* Professor Upamanyu Madhow, University of California - Santa Barbara; Dr. Purush Iyer, Network Sciences Division
- *Equipment Support for Multi-human Multi-robot Interactions,* Professor Dinesh Manocha, University of Maryland – College Park; Dr. J. Michael Coyle, Computing Sciences Division
- *A Medium-Distance Quantum Network with Fiber-Ready Trapped Atomic Ions,* Professor Norbert Linke, University of Maryland – College Park; Dr. Derya Cansever, Network Sciences Division
- *Novel Method for Monitoring the Aging of Missile Propellant Stabilizers, Professor Paul Ruffin, Alabama A&M University;* Dr. James Parker, Chemical Sciences Division
- *Understanding of light based quantum processes in selected biomaterial from the brain, microtubules, and cells,* Professor Robert Alfano, CUNY – City College of New York; Dr. Richard Hammond, Physics Division
- *Charge-separation photodetectors with long carrier lifetime b.ii.(3),* Professor Yong-Hang Zhang, Arizona State University; Dr. Michael Gerhold, Electronics Division
- *Proton dynamics in protic ionic liquids and plastic crystals, including 40 new pKa units beyond OH,* Professor Charles Angell, Arizona State University; Dr. Robert Mantz, Chemical Sciences Division
- *Secure Topological Interference Management for Tactical Wireless Networks,* Professor Syed Jafar, University of California – Irvine; Dr. Derya Cansever, Network Sciences Division
- *Uncertainty-based Mathematical Methods for Simulating Confined, Unsteady Flow Dynamics with Particle Entrainment, Professor Alison Flatau, University of Maryland – College Park; Dr. Joseph Myers, Mathematical Sciences Division*

- *Fractals, Lyapunov exponents, and spectral theory of almost Mathieu operator (AMO) of Jacobi type,* Professor Kasso Okoudjou; University of Maryland – College Park; Dr. Joseph Myers, Mathematical Sciences Division
- *Interfacial Misfit Dislocation Array based Metamorphic Antimonide Buffers for LWIR Detectors,* Professor Ganesh Balakrishnan, University of New Mexico – Albuquerque; Dr. Michael Gerhold, Electronics Division
- *Nanophotonic Devices for Fast and Efficient LIDAR,* Professor Edo Waks, University of Maryland – College Park; Dr. Michael Gerhold, Electronics Division
- *Crisis and Collective Problem-Solving on the Darkweb: Understanding Crisis Information Processing in Hidden Cyber Communities,* Professor Kyounghee Kwon, Arizona State University; Dr. Lisa Troyer, Life Sciences Division
- *In-band Wireless Trust Establishment Resistant to Advanced Signal Manipulations,* Professor Ming Li, University of Arizona; Dr. Cliff Wang, Computing Sciences Division
- *Determination of electrical and geometrical characteristics of mine-like and IED-like targets using new globally convergent inverse algorithms,* Professor Mikhail Klibanov, University of North Carolina – Charlotte; ; Dr. Joseph Myers, Mathematical Sciences Division
- *Organically Controlled Crystal Growth and Phase Selection in Ecologically Diverse, Ultrahard Bio-composites,* Professor David Kisailus, University of California - Riverside; Dr. Stephanie McElhinny, Life Sciences Division
- *Processing-Microstructure-Property Maps for Metal Matrix Composite Developed by Ultrasonic Cavitation,* Professor Arvind Agarwal, Florida International University; Dr. Michael Bakas, Materials Science Division
- *Efficient Computational Models for Simulating Large-Scale Heterogeneous Crowds,* Professor Ming Lin, University of Maryland – College Park; Dr. J. Michael Coyle, Computing Sciences Division
- *Investigation of Laminar-Turbulent Transition for Transonic Boundary Layers using Advanced Computational Tools,* Professor Hermann Fasel, University of Arizona; Dr. Matthew Munson, Mechanical Sciences Division
- *Carrier dynamics and modulation properties of selective area epitaxial quantum structures in dielectric nanophotonic cavities for high speed and energy efficient lasers,* Professor Weidong Zhou, University of Texas – Arlington; Dr. Michael Gerhold, Electronics Division
- *Phononic Effects in Diamond Electronics,* Professor Mitra Dutta, University of Illinois – Chicago; Dr. Joe Qiu, Electronics Division
- *In-operando high-speed microscopy and thermometry of reaction propagation in polymer nanocomposites,* Professor Michael Zachariah, University of California – Riverside; Dr. Ralph Anthenien, Mechanical Sciences Division
- *21st Annual SQuInT Workshop,* Professor Ivan Deutsch, University of New Mexico – Albuquerque; Dr. Sara Gamble, Physics Division
- *Student Travel Support for IEEE S&P 2019,* Professor Yao Liu, University of South Florida; Dr. Cliff Wang, Computing Sciences Division
- *International Workshop on Quantum Network Science,* Professor Saikat Guha, University of Arizona; Dr. Derya Cansever, Network Sciences Division
- *Artificial Intelligence (AI) Embedded Information Assurance (IA) Workshop Proposal,* Professor Sitharama Iyengar, Florida International University; Dr. Cliff Wang, Computing Sciences Division
- *Science of Team Science Conference Grant,* Professor Maritza Salazar Campo, University of California – Irvine; Dr. Edward Palazzolo, Network Sciences Division
- *Workshop on Distributed Reinforcement Learning and Reinforcement Learning Games,* Professor Frank Lewis, University of Texas – Arlington; Dr. Derya Cansever, Network Sciences Division
- *ACM WiSec 2019 Conference, Professor Mohammad Rahman, Florida International University; Dr. Cliff Wang, Computing Sciences Division*
- *Proactive and Autonomous Defensed in Wireless Networks,* Professor Yanchao Zhang, Arizona State University; Dr. Cliff Wang, Computing Sciences Division
- *Student Travel Support for the seL4 summit,* Professor Yao Liu, University of South Florida; Dr. Cliff Wang, Computing Sciences Division
- *Manipulation and Decoherence of Spin-valley Qubits in Monolayer Transition Metal Dichalcogenide Nanostructures, Professor Junxia Shi, University of Illinois – Chicago; Dr. Joe Qiu, Electronics Division*
- *Assessing and Expanding the Limits of Collective Intelligence, Professor Adolfo Escobedo, Arizona State University; Dr. Purush Iyer, Network Sciences Division*
- *Molecular State Readout via Strong Optical Fields, Professor David Patterson, University of California – Santa Barbara; Dr. Paul Baker, Physics Division*

- *Quantum-secure low probability of detection/intercept (LPD/LPI) networks, Professor Boulat Bash, University of Arizona; Dr. Derya Cansever, Network Sciences Division*
- *Entanglement-Assisted Communication and Networking in a Contested Environment, Professor Quntao Zhuang, University of Arizona; Dr. Derya Cansever, Network Sciences Division*
- *Addition of a driver section extension for the UIC High Pressure Single Pulse Shock Tube, Professor Kenneth Brezinsky, University of Illinois – Chicago; Dr. Ralph Anthenien, Mechanical Sciences Division*
- *Acquisition of a Seahorse XFe Analyzer for polymer testing with live cells, Professor Pascal Binda, Savannah State University; Dr. Dawanne Poree, Chemical Sciences*
- *The Impact of Body Size on Resilience in Apis mellifera, Professor Olav Rueppell, University of North Carolina – Greensboro; Dr. Robert Kokoska, Life Sciences Division*
- *Imaging Non-equilibrium Hot Carrier Dynamics in 2D Materials and Their Heterostructures with Scanning Ultrafast Electron Microscopy - Novel Functional Materials, Professor Bolin Liao, University of California – Santa Barbara; Dr. Chakrapani Varanasi, Materials Science Division*

As for all institutions funded through the ARO Core Program, HBCU/MSIs selected for funding were afforded the opportunity to submit add-on proposals to fund high school and/or undergraduate student research apprenticeships through HSAP/URAP. A total of 10 HBCU/MSIs were funded under HSAP/URAP in FY19, totaling approximately $71K (~50/50 mix of PM and Army Education Outreach Program (AEOP) funding). Additional information regarding HSAP/URAP can be found in the Educational Outreach Activities section.

Partnered Research Initiative (PRI)

The PRI Program was established as the next phase of what was previously known as the Partnership in Research Transition (PIRT) Program, which ended in FY16. The focus of the PRI Program is to advance innovative basic research leading to potential technology development in areas of strategic importance to the Army by bringing competitively selected HBCU/MSI research teams into existing ARL Collaborative Research Alliances (CRAs) and Collaborative Technology Alliances (CTAs). The CTAs and CRAs are large collaborative centers focused on developing and transitioning research in Army critical areas.

In FY19, ARL's PRI Program for HBCUs/MSIs continued funding four projects totaling $1.36 million through the CTA/CRA consortia: The New Mexico Institute of Mining and Technology as part of the Multiscale Modeling of Electronic Materials CRA; City College of New York as part of the the Cognition and Neuroergonomics CTA; University of Texas at El Paso as part of the Cyber Security CRA; and North Carolina Agricultural and Technical State University as part of the Materials in Extreme Dynamic Environments (MEDE) CRA. The projects listed below may be funded for up to four years (thru FY20) and are performed in collaboration with ARL and CTA/CRA member institutions to maximize the impact of the research and enhance HBCU/MSI research capabilities.

PRI Title: Defeating the Dark Triad in Cyber-security Using Game Theory
Integrated into Cyber Security CRA
CTA/CRA Collaborating Institution: University of Texas at El Paso
PI: Professor Christopher Kiekintveld
Cooperative Agreement Manager (CAM): Dr. Michael Frame

PRI Title: Material Design Under Uncertainty
Integrated into Multiscale Modeling of Electronic Materials CRA
CTA/CRA Collaborating Institution: New Mexico Institute of Mining and Technology (NMT)
PI: Dr. Yanyan He
CAM: Dr. Meredith Reed

PRI Title: Tailoring Mg-alloy Systems through Composition / Microstructure/Severe Plastic Deformation for Army Extreme Dynamic Environment Applications
Integrated into Materials in Extreme Dynamic Environments (MEDE) CRA
CTA/CRA Collaborating Institution: North Carolina A&T State University
PI: Dr. Jagannathan Sankar
CAM: Dr. Sikhanda Sataphy

PRI Title: Reliability of Neural Activity as an Assay of Cognitive State
Integrated into Cognition and Neuroergonmics CTA
CTA/CRA Collaborating Institution: City College of New York (CCNY)
PI: Dr. Jacek Dmochowski
CAM: Dr. Jon Touryan

DoD Research and Educational Program (REP) for HBCU/MSIs

ARO has administered programs on behalf of OASD(R&E) since 1992. REP aims to enhance research capabilities of HBCUs and MSIs and to strengthen their education programs in science, technology, engineering, and mathematics (STEM) disciplines that are relevant to the defense mission.

Under this program, qualifying institutions were able to submit proposals to compete for basic research grants. In FY19, Funding Opportunity Announcement (FOA) W911NF-18-S-0006 was issued for the DoD REP for HBCUs/MSIs, with 175 proposals identified as eligible under the solicitation. In FY19, 59 grants totaling $23.3 million were made to 18 unique HBCUs, 1 Tribal, and 26 to unique MSIs under the DoD REP solicitation.

Other HBCU/MSI Activities

On 12-13 June 2019, ARO in partnership with the Office of the Under Secretary of Defense for Research and Engineering (OUSD (R&E)) hosted a two day workshop in Research Triangle Park, NC to provide technical assistance on how to do business with DoD and ARO. This event was attended by over 225 registered participants from across the country. Participants (from academic leadership and researchers to sponsored program officials) received assistance in developing competitive proposals in response to DoD funding opportunities including the: DURIP; MURI; Minerva Initiative; Established Programs to Stimulate Competitive Research (EPSCOR); Defense Established Programs to Stimulate Competitive Research (DEPSCOR); and the Science, Mathematics and Research for Transformation (SMART) Program.

This year's workshop moved to a new two day itinerary and a new larger meeting space for an interactive and engaging workshop with dedicated networking breaks and a poster exhibition of DoD HBCU/MSI Centers of Excellence and their innovative research. This expanded format enabled key customers and stakeholders in the HBCU/MSI community to engage with technical Program Managers and subject matter experts from across DoD to help them to have greater knowledge of how to partner with federal agencies for R&D success, how to work with DoD contracting officers (pre-award to post-award), and enhancing HBCU/MSI competitiveness beyond targeted programs. The workshop focused on increasing HBCU/MSI participation in activities throughout the DoD research enterprise, white paper and proposal processes, and highlighting what evaluators consider when reviewing proposals.

Also in FY19, CCDC ARL executed its first-ever HBCU/MSI Undergraduate Student Design Competition with much support from ARO, ACC-APG RTP Division, and several ARL directorates. ARO demonstrated strong technical and operational knowledge helping bring the idea of the Inaugural CCDC HBCU/MSI Student Design Competition into fruition through exceptional execution and program management.

The goals of the competition were to:

- Introduce HBCU/MSI students to Army research and technical challenges and increase student interest in Army science and engineering
- Engage HBCU/MSI students with the Army's technical and operational communities
- Implement ARL's HBCU/MSI engagement strategy
- Stimulate innovation and entrepreneurship

Eleven teams (5 from HBCUs, 6 from MSIs) were selected to compete in the competition in El Paso, TX on 23-25 April 2019. Each team received an $8,000 grant to cover travel costs to El Paso for the poster session and flight demonstration. Just $500 could be used to build a UAV prototype. Mentors from CCDC and its Army Research Laboratory helped students refine their design and ensure their UAV was flight worthy. More than 1,000 local El Paso middle and high school students cheered on the competitors as each team used their 10-minute flight block to maneuver their UAV through a series of challenges on the course at the campus of University of Texas – El Paso. The event was a tremendous success with planning already underway for the 2020 HBCU/MSI Student Design Competition to be held in Chicago, IL.

National Defense Science and Engineering Graduate (NDSEG) Fellowship Program

The NDSEG Fellowship Program is a tri-service program administered by the Air Force Office of Scientific Research (AFOSR), designed to increase the number of U.S. citizens trained in disciplines of science and engineering important to defense goals. ARO supports the NDSEG Fellowship Program along with the Office of Naval Research (ONR) and AFOSR. NDSEG is a highly competitive fellowship awarded to U.S. citizens who have demonstrated a special aptitude for advanced training in science and engineering, and who intend to pursue a doctoral degree in one of sixteen scientific disciplines of interest to the military. NDSEG Fellowships are for years of sponsorship. Fellows are provided full tuition and fees at any accredited university of choice, a monthly stipend very competitive with other top-tier fellowships ($3,200/month), up to $1,200/year in medical insurance, and $5,000 to support travel during the duration of the fellowship.

With the funds made available to the Army to support candidates in FY19, ARO selected 56 NDSEG Fellows from 14 categories relevant to Army fundamental research priorities. These awardees began their fellowships in the fall of 2018. Each of ARO's divisions reviewed the applications assigned to NDSEG topic categories within their particular areas of expertise, and selected fellows whose doctoral research topics most closely align with the Army's missions and research needs. As in past years, with the exception of FY18, the number of Fellows chosen from each discipline was based roughly on the percentage of applicants who submitted topics in that category. The number of fellows chosen from each scientific discipline for the FY19 NDSEG program is shown in Table 2.

Table 2

FY19 NDSEG fellows by discipline. The table displays the number of NDSEG Fellows chosen in FY19, according to topic categories relevant to the designated Army research priorities.

Scientific Discipline	NDSEG Fellows Selected in FY19
Aeronautical and Astronautical Engineering	4
Biosciences & Biomedical Engineering	9
Chemical Engineering	4
Chemistry	4
Civil Engineering	2
Cognitive, Neural, and Behavioral Sciences	5
Computer and Computational Sciences	5
Electrical Engineering	4
Geosciences	3
Materials Science and Engineering	6
Mathematics	2
Mechanical Engineering	3
Physics	5
	TOTAL 56

Education Outreach Activities

All the programs managed by the Army Educational Outreach Program (AEOP) STEM Outreach Office at CCDC Headquarters share one principal purpose: to increase the number of future adults with careers in science, technology, engineering, and mathematics. These programs accomplish this through a variety of mechanisms, including: providing a work/study laboratory experience, sponsoring hands-on science workshops during the summer, showcasing talented young high school scientists at symposia, and supporting student science fairs nationwide. Of these many programs, ARO continued to administer the High School and Undergraduate Research Apprenticeship Programs in FY19 within the ARO Technology Integration and Outreach Division.

During the summer of FY19, 83 students served as apprentices and worked in university laboratories with mentors though the High School Apprenticeship Program (HSAP) and the Undergraduate Research Apprentice Program (URAP). This was a 27% decrease in the number of participants in FY18. These programs are described further in the following subsections.

Undergraduate Research Apprenticeship Program (URAP)

URAP funds the STEM apprenticeship of promising undergraduates to work in university-structured research environments under the direction of ARO-sponsored PIs or their senior research staff serving as mentors. In FY19, URAP awards provided 54 students with research experiences at 41 different universities in 24 different states. Ten (10) of the universities were HBCU/MSIs. ARO invested approximately $109K of the $234K total in the FY19 URAP effort, a mix of ARO core funding and AEOP matching funds.

High School Apprenticeship Program (HSAP)

HSAP funds the STEM apprenticeship of promising high school juniors and seniors to work in university-structured research environments under the direction of ARO-sponsored PIs or their senior research staff serving as mentors. In FY19, HSAP awards provided 29 students with research experiences at 25 different universities in 16 different states. Six (6) of the universities were HBCU/MSIs. ARO invested approximately $43K of the $86K total in the FY19 HSAP effort, which includes ARO core funding and AEOP matching funds.

Local Outreach

- ARO participated in the following additional outreach efforts in FY19.
- North Carolina Science and Engineering Fair: ARO PMs volunteered to judge posters for a special category that presents awards to high school juniors and seniors based upon the overall quality and Army relevance of their projects.
- JSHS National Symposium: scientists from ARO and sponsored PIs attended and judged student posters as well as oral presentations of students that have previously won regional competitions. Winners are awarded various scholarships ranging from $4,000 to $12,000. Sponsored PIs also conducted tours of their labs for JSHS participants.
- Site visits to local and out of state universities that host HSAP/URAP participants: the HSAP/URAP Program Coordinator visited seven (7) host sites in California and New York to monitor program efficacy.
- STEM Fests: ARO joined the RTP STEM, a nonprofit organization that facilitates Science, Technology, Engineering and Mathematics outreach and mentoring opportunities for underrepresented minorities, during their two 2019 Expos/Fairs. Program Managers from ARO in the fields of chemistry, physics, mathematics, environmental, social and life sciences volunteered as speed mentors to an estimated 360 students ranging from grades 5 to 12 at the Frontier building in Research Triangle Park, North Carolina. The Youth Sciences Program Coordinator also staffed displays promoting Army research/technology and the AEOP at the event, including HSAP and URAP.

Scientific Services Program (SSP)

ARO established the SSP in 1957. This program provides a rapid means for the Army, DoD, OSD, and other federal government agencies to acquire the scientific and technical analysis services of scientists, engineers, and analysts from small and large businesses, colleges and universities, academics working outside their institutions, and self-employed persons not affiliated with a business or university. Annual assistance is provided through the procurement of short-term, engineering and scientific technical services in response to user-agency requests and funding. Through the SSP, these individuals provide government sponsors with scientific and technical results and solutions to problems related to R&D by conducting well-defined studies, analyses, evaluations, interpretations, and assessments in any S&T area of interest to the government.

SSP services are currently administered and managed for ARO through Edmond Scientific Company (headquartered in Alexandria, VA), and previously administered and managed by Battelle Memorial Institute (headquartered in Columbus, Ohio). The program was re-competed during FY19 resulting in a new IDIQ award made to Edmond Scientific Company. Edmond's responsibilities include the selection of qualified individuals, universities, businesses, and/or faculty to perform all tasks requested by ARO, and for the financial, contractual, security, administration, and technical performance of all work conducted under the program.

SSP awards tasks in a wide variety of technical areas, including mechanical engineering, computer sciences, life sciences, chemistry, material sciences, and military personnel recruitment/retention. In FY19, 6 new SSP tasks were awarded with 21 modifications to the scope and/or funding of ongoing tasks, in addition to the re-compete and subsequent award of the master IDIQ supporting the program. A summary of the agencies served under this program and the corresponding number of FY19 new SSP tasks is provided in Table 3.

Table 3

FY19 new SSP tasks and sponsoring agencies. In FY19, 6 new SSP tasks were awarded in addition to 21 modifications of the scope and/or funding of ongoing tasks in SSP contracts.

Sponsoring Organization	SSP Tasks
CCDC (formerly RDECOM)	
Army Research Laboratory (ARL)	1
TOTAL: CCDC	**1**
Other U.S. Army	
Combined Arms Support Command (CASCOM)	3
Program Executive Office – Ground Combat Systems (PEO-GCS)	1
TOTAL: Other U.S. Army	**4**
Other DoD	
Defense Logistics Agency (DLA)	1
TOTAL: Other DoD	**1**
TOTAL FY18 New SSP Tasks	**6**

Summary Of Program Funding and Actions

FY19 Research Proposal Actions

ARO PMs receive white papers throughout the year and discuss these topic ideas with the potential investigator to identify any ways the proposed research could better align with program vision and Army needs. PMs then encourage a subset of the white papers to be submitted as full proposals; however, any eligible investigator can submit a full proposal, regardless of PM recommendations. It is rare for a potential investigator to submit a full proposal without first submitting a white paper. Approximately one-third of the white papers received by ARO PMs from academic institutions are ultimately submitted as formal, full proposals. The actions for FY19 extramural basic research white papers and full proposal submissions are summarized in Table 4.

Table 4

FY19 ARO Research Proposal Actions. The status of white papers and research proposals received by ARO within FY19 (i.e., 1 Oct 2018 through 30 Sep 2019) is listed for each scientific division, based on actions for FY19 proposals that were completed on or before 3 Dec 2019. The table reports actions for new-start proposals in the basic research categories: SI, STIR, YIP, HBCU/MSI, MRI, MURI, and DURIP.

	White Papers	Full Proposals				
	Received	Received	Accepted	Declined	Pending	Withdrawn
Chemical Sciences	216	126	39	24	63	0
Computing Sciences	109	41	13	7	20	1
Electronics	149	47	18	14	15	0
Life Sciences	387	75	20	22	32	1
Materials Science	327	70	15	26	28	1
Mathematical Sciences	161	32	14	1	17	0
Mechanical Sciences	162	108	16	35	57	0
Network Sciences	105	76	26	10	39	1
Physics	112	91	26	33	32	0
Tech Integration and Outreach	n/a[3]	186	12	13	161	0
TOTAL	**1,728**	**852**	**199**	**185**	**464**	**4**

[1]White papers are defined as potential research concepts submitted to an ARO Program Manager for discussion and potential submission as a full proposal, in line with the process outlined in the ARO BAA.
[2]A proposal may remain in pending for a variety of reasons, with the chief cause being insufficient funds available to support the research in the same year the proposal was received. In those cases, the proposal can be considered for funding in the subsequent year if sufficient funds are available.
[3]White papers for projects awarded through the Tech Integration and Outreach Division were submitted through OASD(R&E) and/or the ARO division most closely aligned to each proposal's scientific discipline.

Summary of ARO Core Program Budget

The ARO FY19 Core (BH57) Research Program budget is shown in Table 5, below.

Table 5

ARO Core (BH57) Program funding. The ARO Core Program FY19 Budget is listed according to each scientific discipline (Division) or special program. The FY19 Allotment totals shown here are the funds ARO had received and allotted within FY19, regardless of the year of appropriation, based data posted in the General Fund Enterprise Business System (GFEBS) as of 31 Oct 2019 and the corresponding ARO Status of Funds Report.

ARO Core (BH57) Program Type	Division or Program Title	FY18 Allotment
Scientific Disciplines[1]	Chemical Sciences[2]	$9,793,706
	Computing Sciences	$6,485,342
	Electronics	$7,738,000
	Life Sciences	$8,680,368
	Materials Science	$8,775,000
	Mathematical Sciences	$7,369,011
	Mechanical Sciences[3]	$8,872,000
	Network Sciences	$8,587,291
	Physics	$8,761,150
SUBTOTAL: Core Program Funding by Scientific Discipline		**$75,061,868**
Special Programs	Senior Scientist Research Programs	$674,189
	International Offices[4]	$3,174,619
	Technology Integration and Outreach	$1,115,174
	ARL General and Administrative Support	$2,638,544
	In-House Operations	$12,946,073
SUBTOTAL: Core Program Funding by Scientific Discipline		**$20,548,599**
TOTAL	**ARO Core (BH57) Program**	**$95,610,467**

[1]Scientific divisions also received and executed funds through the Army's Congressional Basic Research Initiatives (not shown here; refer to Table 6)
[2]As of FY19, this division includes the Environmental Chemistry program.
[3]The Earth Sciences program was managed within this division in FY19.
[4]Includes funds for research grants monitored through ARO International PMs

Summary of Other Programs Managed or Co-managed by ARO

The FY19 allotments and funding sources for other ARO managed or co-managed programs (i.e, not part of the ARO Core Program), are shown in Tables 6-8.

Table 6

FY19 allotments for other Army-funded programs. . These programs, combined with the ARO Core (BH57) Program elements shown in Table 5, represent all of the Army funds managed through ARO. The FY19 allotments include funds ARO received and allotted within FY19, regardless of the year of appropriation. Data source: ARO 31 Oct 2019 GFEBS Status of Funds Report.

Other Army-funded Program	FY18 Allotment
Multidisciplinary University Research Initiative	$45,828,678
Presidential Early Career Award for Scientists and Engineers	$2,467,744
Defense University Research Instrumentation Program	$9,973,338
University Research Initiative Support	$4,543,240
HBCU/MSI – PIRT Centers (Project H04)	$907,000
Institute for Collaborative Biotechnologies (ICB; Project H05)	$5,773,000
Institute for Soldier Nanotechnologies (ISN; Project J12)[2]	$5,773,000
Institute for Creative Technologies (ICT; Project J08)	$6,196,000
UARC Congressional Support	$3,000,000
Board of Army Science and Technology (BAST; Project C18)	$1,865,000
Small Business Innovation Research (SBIR; Project M40)[1,3]	$3,689,974
Small Business Technology Transfer (STTR; Project 861)[1,4]	$14,738,568
SBIR/STTR Services / Contract Support (Project 720)[5]	$911,839
Basic Research Initiatives – Congressional (Project T14)	$15,000,000
TOTAL: Other Army-funded Programs	**$120,667,380**

[1]Does not show additional funds provided by OSD (see Table 8)

Table 7

OSD direct-funded programs. These funds were allocated directly from OSD to the indicated program. Data source: 31 Oct 2019 GFEBS Status of Funds Report.

OSD Direct-funded Programs	FY19 Allotment
SBIR/STTR (Projects 861, M40)[1]	$499,953
Chemical and Biological Defense Programs (Project BP0)	$1,504,260
HBCU/MSI Research and Educational Program (REP)[2]	$25,665,000
TOTAL: OSD Direct Funding	**$27,669,213**

[1] Does not include additional Army funds provided for SBIR/STTR (see Table 6).

[2] This amount does not include the other Army funds for the HBCU/MSI PIRT Program (see Table 6).

Table 8

FY19 allotment for externally-funded programs. FY19 funds received from sources other than Army or OSD are indicated below. The Other Agencies category totals the funds from a range of DoD and U.S. government agencies, such as the Defense Threat Reduction Agency (DTRA). Data source: GFEBS Status of Funds Reports from 31 Oct 2019 or 30 Sep 2019 (for FY18 funds received in or reallocated for FY19).

External Program	FY18 Allotment
Scientific Services Program (SSP)[1]	$2,152,922
Defense Advanced Research Projects Agency (DARPA)[2]	$112,345,821
Other Agencies (e.g., DTRA)[3]	$163,790,229
TOTAL: External Programs	**$278,288,972**

[1]Includes $117,989 of FY17 funds received in or reallocated for FY18

[2]Includes $8,974,619 of FY17 funds received in or reallocated for FY18

[3]Includes $41,859,647 of FY17 funds received in or reallocated for FY18

Grand Total FY19 Allotment for ARO Managed or Co-managed Programs

Table 9

Summary of FY18 allotment for all ARO managed or co-managed programs. This table lists the subtotals from Tables 6-9 and the grand total FY18 allotment for all ARO managed or co-managed programs. The FY18 allotments include funds ARO received and allotted within that FY, regardless of the year of appropriation (e.g., FY18 allotment includes any FY17 funds received during or allocated for FY18). Refer to Tables 6-9 for data source information.

Program Category	FY19 Allotment
Core (BH57) Programs	$92,778,222
Other Army-funded Programs	$114,477,257
External Program Funds	$250,966,733
OSD Direct-funded Programs	$35,209,827
GRAND TOTAL: (all sources)	**$493,432,039**

Chapter 03

ARO FY19
Success Stories

This chapter provides a brief summary of the ARO Success Stories in FY19, organized by ARO Directorate, Division, and the associated program manager (PM) or other ARO staff. Each success story represents fundamental studies that will also impact one or more ARL Core Competencies.

This background image is from "Demonstration of Non-trivial Topological Properties in Graphene" on page 245.

CHAPTER

03 ARO FY19 Success Stories

Index

ARO FY19 Success Stories with links to ARL Core Technical Competencies.

ARL Core Technical Competencies (CTCs)

The ARL technical strategy provides a comprehensive vision of the future technical landscape and is a critical component of its Research Management and Leadership Strategy. Key aspects of ARL's technical strategy are the seven Core Technical Competencies (CTCs) that guide the laboratory in identifying the scientific, technical, and analytical areas of vital importance to the Army of the future. These CTCs guide the laboratory in identifying and answering critical research questions in support of the Army's strategy for Multi-domain Operations and the required Army Functional Concepts. A brief summary of each CTC is provided in this section.

ARO's programs support each of the CTCs; however, as noted in Chapter 1, ARO's mission represents the most long-range Army view for changes in its technology, with system applications often 20-30 years away. ARO pursues a long-range investment strategy designed to maintain the Army's overmatch capability in the expanding range of present and future operational capabilities.

(M) Materials and Manufacturing Sciences

Research in this CTC drives the discovery and creation of superior materials and devices needed to enable lasting strategic land power dominance. The future Army will require materials with unprecedented properties rapidly manufactured, grown, synthesized, and produced cost-effectively to enable highly mobile, information reliant, lethal, and protected Army platforms. This technology enables the Army to execute real-time, point-of-need design and fabrication thereby increasing agility and logistical efficiency from the microscale to the infrastructure scale.

(C) Computational Sciences

This CTC focuses on advancing the fundamentals of predictive simulation sciences, data intensive sciences, computing sciences, and emerging computing architectures to transform the future of complex Army applications. Foundational research in artificial intelligence and machine learning will enable autonomous cross-domain maneuver warfighting concepts with intelligent agents that rapidly learn, adapt, and reason faster than the adversary to fight and win in contested, austere, and congested environments.

(B) Ballistics Sciences

This CTC focuses on gaining a greater understanding and discovery of mechanisms and on generating concepts and emerging technologies that support kinetic lethality. Knowledge and concepts gained will lead to unprecedented enhancements in weapons range, precision, and lethality for the mounted and dismounted Soldier against a spectrum of manned and unmanned ground and aerial combat systems.

(H) Human Sciences

This CTC focuses on identifying, creating, and transitioning scientific discoveries and technological innovations underlying Human Behavior; Human Capabilities Enhancement; and Human-System Integration that are critical to the U.S. Army's future operational superiority. Foundational research in human agent teaming provides human agent teams with the capability to perform as well as Soldier teams but with greater team resilience, faster, more informed team decision making, and reduced numbers and risk to Soldiers.

(P1) Propulsion Sciences

This CTC focuses on gaining a greater fundamental understanding of advanced mobility and maneuver technologies that enable innovative vehicle configurations and subsystems architectures – critical to the future Army's movement, sustainment, and maneuverability. Foundational research in tactical unit energy independence enables energy-intelligent autonomous squad support systems that lighten the Soldier load, providing a more maneuverable, sustainable, and lethal force and intelligently monitor and distribute power on the move, reducing dismounted Soldiers' cognitive and physical load.

(N) Network and Information Sciences

This CTC focuses on gaining a greater understanding of emerging technology opportunities that support intelligent information systems that perform acquisition, analysis, reasoning, decision-making, collaborative communication, and assurance of information and knowledge. Understanding gained through these research efforts will lead to technological developments that make it possible to manage, utilize, and maintain trust in information flows and geospatial situational awareness within the battlespace.

(P2) Protection Sciences

This CTC focuses on gaining a greater understanding and discovery of mechanisms and generating concepts and emerging technologies that support protection systems that adapt to evolving threats, and the mechanisms of injury affecting the Warfighter. Foundational research in understanding and manipulating the physics of failure will lead to technologies that enable a broad array of resilient kinetic and non-kinetic protection systems and focuses on precise and accurate knowledge of materials/system failure for protection overmatch.

Success Story	Associated ARO PM/staff	Pg #	M	C	B	H	P1	N	P2
Engineering Sciences Directorate									
Electronics Division									
Radio-frequency Device Applications of a Topological Electronic State of Matter	Harvey	45	●	●				●	
Living Semiconductor Devices are Created for Extraordinary Control of Sub-cellular Functionality	Harvey, Qiu	48				●			●
A Versatile Photonic Platform for Medical Imaging and Beyond	Gerhold, Clark	51	●						
Colloidal Quantum Dot Photodetectors for Low-Cost/High Performance Imaging	Gerhold, Clark	52	●						
Oxide-Free Vertical Cavity Surface Emitting Lasers Demonstrate Superior Thermal Performance	Gerhold	55	●					●	
From Slow-Light Laser to Enhanced Autonomous	Gerhold	58	●					●	
Specialized Materials for Next-Generation Integrated Circuits	Qiu, Varanasi	62	●	●					
Wafer-Scalable, Aligned Carbon Nanotube Transistors Exceeding 100 Ghz	Qiu	64	●					●	
Materials Sciences Division									
Self-Assembling Soft Matter at Liquid Interfaces	Runnerstrom, Prater (retired)	67	●						●
Designing Materials That Respond to Their Environment	Runnerstrom, Poree, Prater (retired), Stepp	70	●						●
Motif Structures in Polymer Nanocomposites	Stepp, Cole	73	●	●					
Elastic Wave Cloaking	Stepp, Cole	76	●						●
Polar Skyrmions in Advanced Materials	Varanasi	79	●	●				●	
Materials with Extraordinary Spin/Heat Coupling	Varanasi	81	●	●				●	
Technical Foundation Established for Synthesis of Advanced Coatings and Energetics via Dusty Plasmas	Bakas, Stepp, Parker	84	●		●				
Means of Inducing Ductility into High Strength Brittle Materials Discovered	Bakas, Stepp	86	●						●
Mechanical Sciences Division									
The Inception of the "Information Engine"	Stanton	89	●	●				●	
Complex Emergent Behavior in Smart Active Particles (Smarticles)	Stanton	92	●						
Understanding Galloping Instabilities of Rectangular Cylinders – Towards Drag Reduction for Precision Airdrop Systems	Munson	96							●
Unmasking Phantom Yaw – Vortex Asymmetry on Slender Bodies at High Angle of Incidence	Munson	99			●				
Enhancing Energetic Materials Performance through Surface Chemistry	Anthenien	102			●		●		
Developing Novel Methods for Probing the Chemical Kinetics of Army Relevant Fuels	Anthenien	104					●		

Success Story	Associated ARO PM/staff	Pg #	M	C	B	H	P1	N	P2
Functionalizing Fiber Interfaces for Controlled Load Distribution	Ford, Anthenien	106	●						●
Predicting The Deformation Behavior of Ultrahard Lightweight Ceramics	Ford, Anthenien	108	●						●
Imaging The Physical Controls on Rock Debris Surface Properties with a Novel 3D Reconstruction Method	Barzyk	110		●				●	
Dust Modeling To Mitigate Hazards	Barzyk	113		●				●	
Information Sciences Directorate									
Computing Sciences Division									
Transforming 3D Reconnaissance Data into Geospatial Intelligence	Coyle	117		●				●	
High-Performance Static and Streaming Tensor Factorization Algorithm	Coyle	119		●				●	
Automatic Data Triage for Better Cyber Defense	Wang	122		●				●	
Establishing Models and Metrics for Cybersecurity Dynamics	Wang	124		●				●	
Brain Computer Interface: First Cross-Monkey Message Decoding	Krim	126		●		●			
Real-time Multimodal Event Detection	Krim	128		●				●	
Systematically Studying Backdoor Attacks on Deep Neural Networks	Fields, Wang	130		●				●	
Mathematical Sciences Division									
Technologies to Target Sleep Disruption in PTSD	Pasour, Gregory	132				●			●
Understanding the Skin Microbiome	Pasour, Kokoska	136				●			●
Making Feasible the Modeling of Many-Electron Materials for Engineering Design	Myers, Stepp	139	●	●					
Optimal Assignments through Perfect Graph Coloring	Myers	141		●				●	
Machine Learning Advances Acknowledged by the Test of Time	Myers	143	●	●					
Topological Data Analysis for Decision-making, System Design, and Material Performance	Myers	145		●				●	
Rapid Computation of Stochastic Processes in Electronic Components	Lavine	148		●				●	
Optimal Assignments through Perfect Graph Coloring	Lavine	149		●				●	
Network Sciences Division									
Scalable Universal Quantum Computing and Networking Using Continuous-Variable Entangled Photonic Graphs	Cansever	151						●	
Ordering for Hypothesis Testing and Beyond	Cansever, Ulman	153						●	
Effective Crowdsourcing	Iyer	155				●		●	
Algorithmic Game Theory	Iyer	157				●		●	
Time-Varying Actuation and Interconnection In Network Systems	Cansever	159						●	

Success Story	Associated ARO PM/staff	Pg #	M	C	B	H	P1	N	P2
Computational Methods For Large-Scale Interconnected Systems With Continuous And Discrete Parameters	Cansever	160						●	
Building a Novel Basic Research Program for Mind-Body-Community Connections	Palazzolo	163				●		●	
Computational Social Science as a Tool for Counterterrorism	Palazzolo	165		●		●		●	
Technology Integration and Outreach Division									
Inclusion of Community College Students in the 2019 URAP	Ardouin, McElhinny	168				●			
ARO Leverages Army Assets In Support Of Local STEM Outreach Event For Underrepresented And Underserved Students	Ardouin, Doss	171				●			
Army STTR Special Topics and Industry Day	Smith, Zachery, Caccuitto, Fox, et. al.	174						●	
STTR Phase 3 – Big Open-Source Social Science (BOSSS)	Smith	175				●		●	
CCDC ARL and ARO Holds First HBCU/MSI Undergraduate Student Design Competition	Huff	178	●	●	●	●	●	●	●
ARO Hosts DoD Workshop For Historically Black Colleges And Universities (HBCUs) And Minority-Serving Institutions (MSIs)	Huff	179	●	●	●	●	●	●	●
ARO Special Programs									
REAPR - Innovative ES/EA Suite Extends to Airborne Platforms	Fox, Ulman	181		●	●			●	●
Scalable Manufacturing of Graphite Yarn via Wet Spinning Process	Fox, Mantz	184	●				●		●
Physical Sciences Directorate									
Chemical Sciences Division									
The First Truly Versatile Polymer Electrolyte ionomer/membrane System	Mantz, Stepp	186	●				●		
Catalyst-Free Synthesis of Ammonia from Nitrogen and Water Using Plasma Electrolysis	Mantz	189	●				●		
Real-Time Ultra-Trace Detection of Organics from Environmental Matrices	King, Mantz	192		●					●
Urban Films as Active Environmental Interfaces	King, Mantz	194		●					●
Two-electron Reduced Density Matrix Methods f or Advanced Computational Chemistry	Parker	198	●	●					
Synthesis of Amorphous Polynitrogen in Cold Liquid Plasma	Parker, Mantz	200	●		●				
Research Integrating Chemistry and Synthetic Biology Led to New BioBit™ Educational Platform	McElhinny, Poree	203	●						
Novel Method for Achieving Controlled Polymer Stereochemistry for Emergent Material Properties	Poree	206	●						
Increasing Catalytic Efficiency with Single Atom Catalysts	Poree	209	●						●

Success Story	Associated ARO PM/staff	Pg #	M	C	B	H	P1	N	P2
Rapid Detection and Identification of Biological Events	Poree	211	●						●
Life Sciences Division									
New Computational Models for Predicting Adversarial Collective Action	Troyer	213		●		●		●	
Institutional Determinants of Emergent Threats to Overmatch by Near-Peer Powers	Troyer	218				●		●	
Supercharging Protein Assembly for Advanced Biotemplated Materials	McElhinny	223	●						●
Research Integrating Chemistry and Synthetic Biology led to new BioBit™ Educational Platform	McElhinny, Poree	225	●						
Blood Chemistry and Surviving Severe Trauma	Strand	228							●
Advancing Understanding of Neurodegeneration Using Single Cell Organisms	Strand	230							●
Bottom-up Construction of Biofilms and Microbial Community Structures	Kokoska	233	●	●					
Screening of Extremophilic Microbial Communities for New Antimicrobials	Kokoska	237							●
New Tool for Seeing the Inner Workings of the Brain	Gregory	239				●			
Emerging View of Vascular Control in the Brain	Gregory	242				●			
Physics Division									
Demonstration of Non-trivial Topological Properties in Graphene	Baker, Ulrich	245	●	●				●	
Demonstration of Non-trivial Quantum Speed-up	Baker, Gamble	248	●	●					
New Instrumentation to Reveal Obscured Electrical Hall Currents	Ulrich	251	●	●					
Demonstration of Non-trivial Topological Properties in Graphene	Ulrich, Baker	253	●	●				●	
Photonic Routing	Ulrich, Hammond (retired)	257	●	●				●	
Supersymmetric Laser Arrays	Ulrich, Hammond (retired)	259	●						
Light-Matter Entanglement Over 50 km of Optical Fiber	Gamble, Govindan	262		●				●	
Quantum Logic Clock	Gamble, Govindan	265		●				●	
University Affiliated Research Centers (UARCs)									
ICB Microbial Fuel Cell Research Leads to Serendipitous Discovery of a New Class of Antimicrobial Compounds	Burgess, Kokoska	268	●			●			●
3D-Printed Shape-Shifting Soft Robots that Can Crawl, Jump and Grab	Burgess, Kokoska	271	●			●			●
Multimaterial Fiber Ink for 3D-Printed Devices that can Sense, Communicate and Store Energy	Burgess, Kokoska	273	●				●	●	

Biotronics Program

Engineering
Sciences
Directoriate

- **Electronics Division**
- Material Sciences Division
- Mechanical Sciences Division

Current Program Scientific Objectives

01

Exploit the unique capabilities of electronic sensing to understand and control in nano-scale detail the interactions within and among cellular and sub-cellular constituents, that if successful will make significant enhancements in Soldier resilience, cognition, performance, and resistance to chemical and biological agents

02

Develop comprehensive models of sub-cellular processes which include electrical and Electromagnetics effects at the nano-scale, that if successful will enable a new understanding of the cellular interactions and their impact on tissue and organ level properties, and potentially lead to new clinical and pharmacological treatments for the Soldier

Program Manager

Dr. James Harvey

Program Manager (Acting), Biotronics
Electronics Division
ARO Engineering Sciences Directorate

Dr. Harvey completed his undergraduate studies at the U.S. Military Academy, receiving his B.S. in engineering in 1964. He received an M.A. in Physics at Dartmouth College in 1971. He trained as a physicist at Lawrence Livermore National Laboratory, receiving his Ph.D. in applied science in 1991 from the University of California - Davis.

SUCCESS STORY

Radio-frequency Device Applications of a Topological Electronic State of Matter

This ARO initiative resulted in the **discovery of new electronic properties of a material known as a Dirac semimetal**, which is expected to enable a new generation of electronic devices for the future Army that are smaller, faster, and require less power, thereby reducing the cost, size, and weight of radar, radio, and electronic warfare systems.

Challenge

Today's electronic devices, whether for digital or analog applications, are rapidly approaching performance limits that are set by the fundamental limitations of the current generation of electronic materials. At the same time, demand for greater device performance is driving

This success supports these ARL Core Technical Competencies:

Network and Information Sciences

Materials and Manufacturing Sciences

Computational Sciences

device structures to smaller dimensions and faster speeds of operation, with dissipated power a major constraint. For example, transistors face enormous difficulties because they cannot adequately contain and control sufficient charge densities within structures of a few-atom dimensions. While some of the most intensely researched new electronic materials, such as the 2D structures (i.e., graphene, chalcogenides, etc.) may provide potential solutions, there are significant constraints that limit their performance when compared with the larger devices of Si or III-V semiconductors.

Action

Dr. James Harvey, the program manager of the Electromagnetics and RF program, previously identified and began supporting research at the University of California at Santa Barbara with Professors Robert York and Susanne Stemmer on molecular beam epitaxy (MBE) deposition of high quality Barium Strontium Titanate epitaxial films for tunable RF filters. Professor Stemmer is one of the premier pioneers in MBE growth and had been highly successful with a MURI on complex oxides, a very difficult material for MBE. After a project review, Dr. Harvey was encouraging the team to speculate on what the next advances in epitaxial thin films would provide. The discussion turned to the new interest in Dirac semimetals, in particular Cd_3As_2, which had recently been experimentally shown to be a 3D Dirac semimetal, due to very high potential mobilities and high charge densities. The high mobility arises in part from the band structure which has a Dirac point, at which the carriers become theoretically massless. Dirac points in Cd_3As_2 occur only at specific values of momentum. The Dirac semimetal is essentially a 3D analog of graphene. They speculated that 2D MBE deposition could significantly change the band structure of the 3D Dirac semimetal in a way to make it more accessible to device application.

Dr. Harvey recognized the novel opportunity to combine the expertise of the leading researcher into MBE thin film growth of complex electronic materials with a pioneer in innovative RF device concepts to realize the promise of this new form of a topological electronic material. The resulting cross disciplinary approach is believed to be the first investigation of this material with equal contributions from the fields of device physics and materials growth.

Result

Professor Stemmer demonstrated the first MBE deposition of high quality Cd_3As_2 thin films supporting quantum Hall effect states. Her group was the first in the U.S. to report the observation of quantum Hall states in a Dirac semimetal. Her experiments demonstrated very high mobilities (~20,000 cm^2/Vs at room temperature). Her group was the first to demonstrate field-effect transistor structures in Cd_3As_2, with modulation of the current with gate voltage. Her experiments were the first to demonstrate conclusively that the Dirac nodes became gapped in the thin film due to quantum confinement and that the surface states were 2D, topologically protected states which screened the bulk states. The gapped bulk states with high mobility surface states enables the gate voltage control of the current in the field-effect transistor (FET) channel (Figures 1-2). The Fermi energy lies within the gap between the valence band and conduction band in the bulk states, while it can lie in the conduction band for the topologically protected Dirac states. Current densities exceeded 10 A/mm at a sheet carrier density of $5x10^{12}cm^{-2}$ and contact resistances were less than 10^{-8}ohm cm^2. In combination with a Fermi velocity of ~$1.5x10^6$ m/s, which is 50% higher than graphene and 3-10 times higher than for most semiconductors, topological insulators, or other semimetals, this makes cadmium arsenide highly promising for RF device applications.

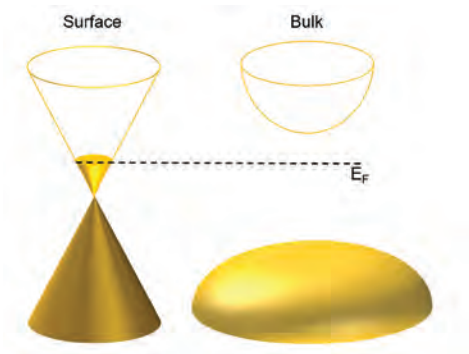

Figure 1: Schematic of the band structure of the bulk and surface states in the Cd_3As_2 thin film, showing the Fermi energy level marking the top of the carrier fill in the bands. The electrons partially filling the conduction band of the surface states can be easily thermally excited into empty energy levels, allowing conduction. The electrons filling the gapped bulk states have nowhere to find empty levels in the gap, so they don't conduct (unless they thermally jump the bandgap).

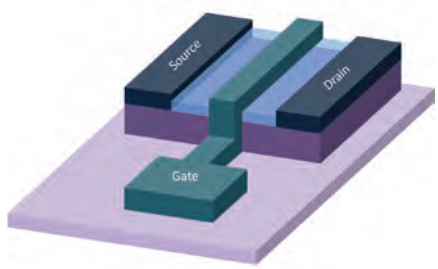

Figure 2: Schematic of the FET structure.

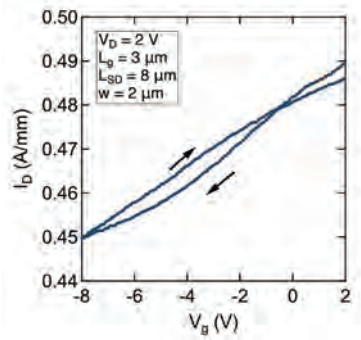

Figure 3: Gate voltage vs drain current curves for the FET structure at room temperature, showing the modulation of the drain current with gate voltage and the absence of saturation in the current.

Results

- Discovery of MBE processing conditions for high quality Cd_3As^2 thin films pointing to low cost, high volume fabrication technologies integrated with standard electronic processing techniques
- Validation of quantum Hall effect in thin films of a 3D Dirac semimetal, indicating that the electrons can be modulated with electric fields in the same manner as conventional transistors, potentially enabling new generations of lighter and less power-intensive electronics
- First demonstration a field-effect transistor with a 3D Dirac semimetal with extremely high mobility, carrier velocity, and charge density and low contact resistance for new device structures supporting faster, smaller, and less expensive radar, communications, and EW electronic systems
- Key step toward topological devices enabling wholly new functionality, potentially opening the door to a new paradigm of low-power electronics

Professor Stemmer was able to show by temperature effect studies that one reason for the low modulation was the screening of the bulk states by the high current densities in the surface states, so that the bulk current was not modulated by the gate voltage. The main reason, however, is the presence of trap states in the gate dielectric. Improving the gate dielectric will increase the current modulation. The temperature dependences of the FET transport shown by Professor Stemmer clearly indicate that the relatively low modulation of the channel current is due to electrostatic screening of the carriers in the bulk states of the channel by the gapless surface states and due to trap states at the interface (Figure 3).

The Way Ahead

Professor Stemmer will address the electrostatic screening by depositing thinner film channels, which should confine and therefore increase the bulk state energy gap, or by epitaxial strain. She will address the problem with the dielectric by investigating alternatives such as BN, which should have no trap states. The MBE FET experiments open the potential for the integration of Dirac semimetal with convention semiconductors in an epitaxial heterostructure for new device concepts and for new device concepts based on switching between topological states. The results of this work have been incorporated in a DARPA program, in an OSD Vannevar Bush Fellowship project, and in a seminar at CCDC ARL. Entirely new opportunities are also opened by the MBE results. Theoretical speculation is that breaking time-reversal or inversion symmetry, for example by incorporating magnetic atoms in the crystal lattice, would change the Dirac semimetal in to a Weyl semimetal, which would open applications in spin devices, chiral carrier states, and even the possibility of an exciting new technology: "chiraltronics."

SUCCESS STORY

Living Semiconductor Devices are Created for Extraordinary Control of Sub-cellular Functionality

This ARO initiative resulted in the **first creation of a living semiconductor device for unprecedented control of sub-cellular electrical processes** in vivo to enable future biotechnologies to treat injuries on site and at the molecular level and to provide resistance to disease and environmental agents, to improve physical resilience, and to improve cognition.

Challenge

Observation and interrogation of sub-cellular biological processes with nano-scale resolution and in living cells are extremely difficult. The bio-chemical processes within a cell are almost entirely moderated by electrical based signaling between organelles, other sub-cellular components, and external bio-based entities in the near cellular environment. However, direct electrical measurement and interrogation must be minimally invasive to preserve the living nature of the cell and its responses. The nanometer scale of the organelles and sub-cellular elements requires nanoscale measurement and probing. The aqueous nature of the cellular material degrades and distorts electrical signals, yet the stochastic complex inter-cellular environment requires high signal to noise measurement, hence these factors a major challenge in this research area.

Action

Dr. Harvey attended a talk by Professor Bozhi Tian of the University of Chicago sponsored by OSD, which focused on recent results in developing interfaces with cells, implantable new biomaterials, and artificial cells. Dr. Harvey was formulating a new electronics research program area in Biotronics, concentrated on the capabilities of advanced nanoelectronic concepts to provide unique nanoscale measurement abilities addressing the electric interactions within a cell and among organelles and new capabilities to modulate bioelectric processes within a cell. He recognized that Professor Tian's research approaches could be focused on the internal bioelectric processes within a cell to obtain new insight into the intracellular biological functionalities. Dr. Harvey worked with Professor Tian to formulate new approaches to intracellular electrical measurement and modulation based on the nanoelectrical devices aimed at new cellular discoveries. The resulting proposal for the exploration of the organelle level, bioelectric information processing using nanoscale semiconductor materials and devices as probes was very promising.

Result

Professor Tian has created three entirely new hybrid biotronic devices which use biological material to make semiconductor nanostructures, which are internalized within the cell and/or connected to the cells through membrane proteins. These are literally living semiconductor devices for non-genetic optical stimulation of cell functionality.

This success supports these ARL Core Technical Competencies:

Human Sciences

Protection Sciences

This success was made possible by the following ARO S&Es:

- Dr. James Harvey, ARO Electronics Division
- Dr. Joe Qiu, ARO Electronics Division

Results

- First creation of living semiconductor-biomaterial hybrid cells with potential capabilities to electrically control heart and nerve cells at subcellular scales to protect or heal the Soldier
- Demonstrated unprecedented capability to modulate subcellular functionality in living cells, enabling the study and understanding of cellular processes affecting physical resilience, resistance to disease and environmental agents, or to modulate or restore organ activity
- Researcher wins runner up essay for the Science & PINS Prize for Neuromodulation, thereby promoting Army research to the scientific community and to attract academic scientific interest to Army-relevant studies

Professor Tian synthesized nanofibers of poly-(3-hexyl thiophene), a polymer known as P3HT, with a direct bandgap (making it a potential semiconductor). He showed that they have mechanical and morphological properties compatible with the extracellular matrix (ECM - the large macromolecular network providing structural and biochemical support of the cell). He incorporated the P3HT nanofibers into the ECM surrounding a cancer cell. The P3HT nanofibers are photothermally active due to their direct bandgap. Professor Tian demonstrated that he could optically stimulate the P3HT to control the temperature in a nanoscale spot near an ion channel (TRPV1 – a protein acting as an ion channel in the cell membrane). The ion channel was activated by the localized heating and opened to transport Ca^{2+} ions into the cell, where they stimulated local mitochondria to produce Caspase 9 (an enzyme). The calcium ion signaling also disassembles focal adhesions in the cell membrane (assemblies of proteins) into other Caspase proteins. This is the first time mitochondria and Caspase signaling has been modulated photo-thermally. The Caspase enzymes and proteins are involved with apoptosis (cell death), immune response, and inflammation. This work enables the photo triggering of intercellular functions and new insights into the control of calcium signaling and bioenergetics at the organelle level.

Professor Tian seeded cardiac myofibroblasts (the cells supporting cardiac cells) with specially textured silicon nanowires, which are easily internalized into the myofibroblasts (Figure 4). The internalized silicon nanowires enable a photoactivation of Ca^{2+} ions in different regions of the myofibroblasts, which transmit the ions to surrounding cardiomyocytes. This enables the resolution of a long standing question of the electrical activity between myofibroblasts and heart muscle cells when in vivo. These integrated hybrid cells enable electrical stimulation with subcellular resolution without interfacing synthetic and rigid electronic devices and open the possibility for future intra-cellular cardiac pacemakers.

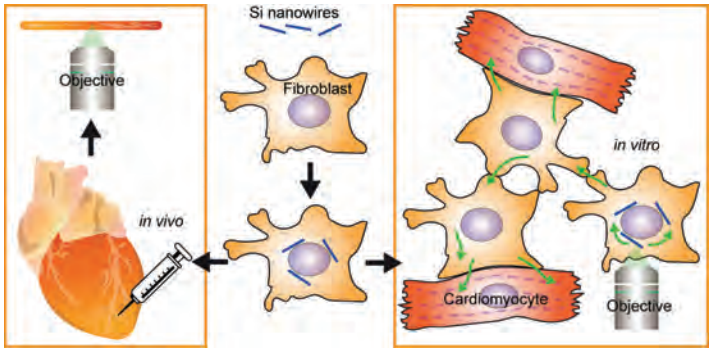

Figure 4: Silicon nanowire-integrated fibroblasts serve as a biophysical tool to probe the subcellular signal propagation in cardiac cells, both in vitro (right) and in vivo (left).

Professor Tian also isolated oligodendrocyte progenitor cells (OPC's) in vitro. OPC's are precursors which transform into oligodendrocytes. The OPC's were seeded with silicon nanowires, which the OPC's internalized. The OPC's were then placed with neural cells. The OPC's differentiated into oligodendrocytes with internalized nanowires, in contact with the neurons. The oligodendrocytes were optically activated, producing a calcium ion flux into the neuron. This enables a highly spatially resolved non-destructive technique for optical stimulation of nerve cells and the investigation of intracellular transient calcium ion flows and the formation of myelin insulating sheaths around axons.

For the first time semiconductor-integrated cells, literally living biotronic devices, were demonstrated providing an unprecedented capability to modulate cells in vivo for control of cellular functionality and the investigation of intra-cellular activity.

Way Ahead

Semiconductor-biomaterial hybrid devices promise new understanding of intracellular electrical activity. Planned research will leverage these devices and internalized semiconductor nano-structures to measure the electrical pathways in the cell and the effect of stimulation on localized areas of mitochondria. These research results are being transitioned to CCDC-ARL via the participating ARL S&E's. They will be briefed to the Army Medical Research and Material Command laboratories and DARPA Biological Technologies Office. The understanding of bioelectric intracellular functionality has the potential to impact Soldier lethality through unprecedented advances in Soldier health and bio-protection, Soldier resilience, Soldier performance, and Soldier cognition.

Electronics Sensing Program

Current Scientific Objectives

01

Explore mid-infrared photodetector heterostructures, processing techniques, and architectures to enhance detectivity for mid-wave and long-wave IR, that if successful will enable lower cost and more flexible operating temperatures for HgCdTe (nightvision) detectors

02

Investigate promising photonic sensing techniques (UV to IR), usually involving intensity enhancements and possibly nonlinear interactions, to enhance the capabilities of both active and passive sensing modalities, that if successful will result in sensors with greater range, resolution, and specificity for Army photonics-based systems

Program Manager

Dr. Michael Gerhold

Program Manager, Optoelectronics
Program Manager (Acting), Electronics Sensing
Electronics Division
ARO Engineering Sciences Directorate

Dr. Gerhold completed his undergraduate studies at Purdue University, receiving his B.S. in Electrical Engineering in 1992, as well as a M.S. in Electrical Engineering in 1994. He received his Ph.D. in Electrical Engineering from the University of Michigan in 1999. He came to ARO in 1999 as the Program Manager for Optoelectronics.

This success supports these ARL Core Technical Competencies:

Materials and Manufacturing Sciences

This success was made possible by the following ARO S&Es or Program Specialists:

- Dr. Michael Gerhold, ARO Electronics Division
- Dr. William Clark (retired), ARO Electronics Division

SUCCESS STORY

A Versatile Photonic Platform for Medical Imaging and Beyond

ARO funding led to the **creation of whispering gallery mode photonic sensors for use in photoacoustic imaging and sensing** that is transitioning for potential commercialization.

Challenge

Ultra-sensitive sensors and transducers are of great importance not only to biomedical research and clinical diagnostics, but also to night vision, environmental sensing for situational awareness and many other fields. The ability to respond to trace amounts of changes in systems, especially in solution with target molecules, an ecological environment, electromagnetic waves, magnetic signals, or infrared radiation, is a significant challenge. The desire is to have a simple, inexpensive and accurate sensing system with real-time and in-situ detection capability.

Action

The former Electronic Sensing program manager, Dr. William Clark, proactively identified a promising young researcher with innovative ideas in high-quality optical resonators, Professor Lan Yang of Washington University in Saint Louis, and she was selected to receive a PECASE award to support her work. During the course of the study, she discussed with Dr. Clark about expanding the scope of her work to night vision; as an expert in optoelectronics, he provided feedback and discussed with her the parameters that are critical for night vision, which led Professor Yang to explore the use optical resonators for ultrasensitive detection of physical matters, such as molecules, proteins or particles. Through Dr. Clark's proactive program management and discussions with her about various promising approaches, Professor Yang also began a unique investigation of the Whispering-Gallery-Mode (WGM) resonators for ultrasensitive detection of infrared radiation. By making use of the thermal changes induced by incident IR signals, the WGM resonator could serve as a transducer that measures a signal that triggers the changes in the resonator itself.

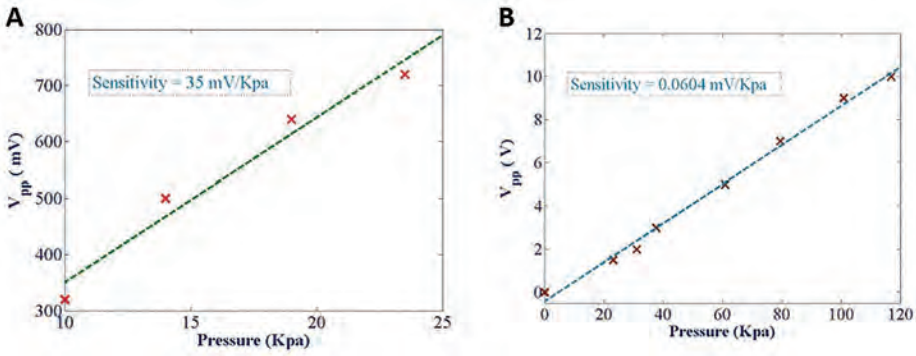

Figure 1: Response of a packaged WGM microtoroid resonator sensor (A) and a commercial Hydrophone (B) to external acoustic pressure.

Result

Professor Yang's ARO funded research efforts demonstrated the WGM resonator not only to be a superior sensor for direct detection of subjects probed by light but also an excellent transducer to indirectly measure an object that could trigger changes in the resonator structure. Professor Yang's team also initiated a collaboration with Dr. Igor Savukov, an expert at Los Alamos National Laboratory, and successfully demonstrated a new ultrasensitive magnetometer composed of an on-chip WGM resonator actuated by a micro-magnet. The high sensitivity, broad dynamic range, as well as the small footprint of the chip-scale sensor makes the WGM magnetometer a promising candidate for magnetic sensing. Furthermore, by measuring the physical changes of the resonator induced by the targets of interest, Professor Yang's group also demonstrated ultrasound sensing for photoacoustic imaging. The physical mechanism lies in resonance changes in the resonator due to the elasto-optic effects induced by the incoming ultrasound. Currently the size of the piezoelectric (acoustic) transducer used to detect ultrasound signal generated by light-induced thermoelastic effects in biological tissues to form images sets the bottleneck to improve resolution in the current photoacoustic imaging systems. Decreasing the size of the detector will make it easier to approach the sensing sites and therefore improve signal-to-noise ratio, and the preliminary data from Professor Yang's group show that high-Q WGM micro-resonators exhibit much higher sensitivity than commercially available acoustic wave transducer. Figure 1 shows a comparison of the response of the WGM ultrasound sensor with that of a commercially available hydrophone.

Way Ahead

In the summer of 2019, Professor Yang and her team successfully demonstrated the readiness of her sensor technology for imaging applications. With the seed funding from industrial partners, a startup company was formed to develop this sensing technology. Professor Yang will be taking a partial sabbatical serving as the Chief Technology Officer of the company. In addition, two of her former students have joined the company to help push forward the WGM technology, aiming to develop disruptive sensing technologies for medical imaging and beyond.

Results

- ARO PECASE program resulted in follow-on research that demonstrated extremely sensing thermal imaging and photoacoustic sensing
- Entrepreneurial effort underway that focuses on development of the improved ultrasound imaging capabilities

SUCCESS STORY

Colloidal Quantum Dot Photodetectors for Low-Cost/High Performance Imaging

ARO funded research demonstrated **interband colloidal quantum dot mid-infrared photodetectors and cameras** that may lead to more flexible operating temperatures for nightvision detectors.

This success supports these ARL Core Technical Competencies:

Materials and Manufacturing Sciences

Challenge

The ability to utilize non-traditional materials and synthesis techniques such as colloidal quantum dots produced by wet chemistry techniques to achieve high operating temperature (HOT), high performance photodetectors has been a major research question for the past 3 decades. Colloidal quantum dots (CQDs) have intriguing

properties such as an easily tunable optical bandgap and low- or zero-dimensional quantum confinement enhanced absorption and emission properties. The challenge is to demonstrate CQD based photodetectors that operate at higher temperatures, at faster response times, and much lower cost than other semiconductor detectors.

This success was made possible by the following ARO S&Es or Program Specialists:

- Dr. Michael Gerhold, ARO Electronics Division
- Dr. William Clark (retired), ARO Electronics Division

Action

Electronic Sensing program manager Dr. Michael Gerhold saw the opportunity for low-dimensional colloidal materials in 2006 when he funded a research opportunity to develop novel solar cell devices based upon PbSe CQDs. ARO's early investments with Professor Jian Xu of Pennsylvania State University spawned other major efforts that advanced IV-VI and II-VI based colloidal materials. Dr. Gerhold also received a unique white paper from Professor Philiippe Guyot-Sionnest of the University of Chicago to study ligand exchange mechanisms to improve carrier transport thru CQDs. At first, Dr. Gerhold was hesitant to support the proposed effort due to the limited success demonstrated to date; however, he was compelled by the strong chemistry expertise that Professor Guyot-Sionnest brought to the scientific challenge. Dr. Gerhold continued to pursue the concept by inviting Professor Guyot-Sionnest to speak at a conference he organized annual at SPIE Photonics West known as the Low Dimensional Quantum Dot and Nanowire Semiconductor Devices meeting. Professor Guyot Sionnest was beginning to explore synthesis of HgTe dots that showed improved luminescence quantum yield over other mid-infrared dots. Dr. Gerhold also shared the white paper with Dr. James Parker of the ARO Chemistry division; simultaneously, DARPA decided to provide Professor Guyot-Sinnoest with a seedling effort to explore the fundamental properties of HgTe CQDs and their suitability for photodetectors.

The DARPA seedling results set the stage for a subsequent ARO Electronics Division proposal focusing on incorporation of the advanced colloidal dots into photodetector regimes. The novel effort proposed to study, and ultimately control the carrier lifetimes of the quantum dots, in addition to the effect of surface modification on the doping level of the quantum dots. Primary emphasis was given to studying mercury and cadmium chalcogenice systems. This project set the stage for the first full evaluation of the improved quantum dots for electronic sensing of mid-infrared photons.

Results

- ARO funding resulted in high profile demonstration of first mid-IR photodetectors based upon colloidal quantum dots
- Careful synthesis and processing studies led to the discovery of core-shell quantum dot thin films

Result

The first main results of this work demonstrated the first mid-infrared quantum dot detectors. Mr. John Roberts did the bulk of this work as an undergraduate (working closely with Professor Guyot-Sionnest), and his results showed record detectives of $3x10^{11}$ Jones and 45% external quantum efficiency at low temperature with 1010 Jones at thermoelectric cooled temperatures (220K). These advances helped Mr. Roberts subsequently receive an NDSEG graduate fellowship to continue his Ph.D. studies. The improvements were based upon improved doping processes using cation exchange with Ag+ ions to achieve high hole doping profiles. High device fabrication yields of 100% were obtained with new doping processes that had only 20% performance variability. Such advances led to systematic studies in improved light trapping structures (including the use of plasmonics and resonant cavities). Eventually this led to demonstration of a scanning imaging system that approached the performance of more expensive, epitaxial InSb single crystal imagers. And, more potential improvements are possible to exceed the current results. The doping studies led to understanding the absolute positions of the electronic

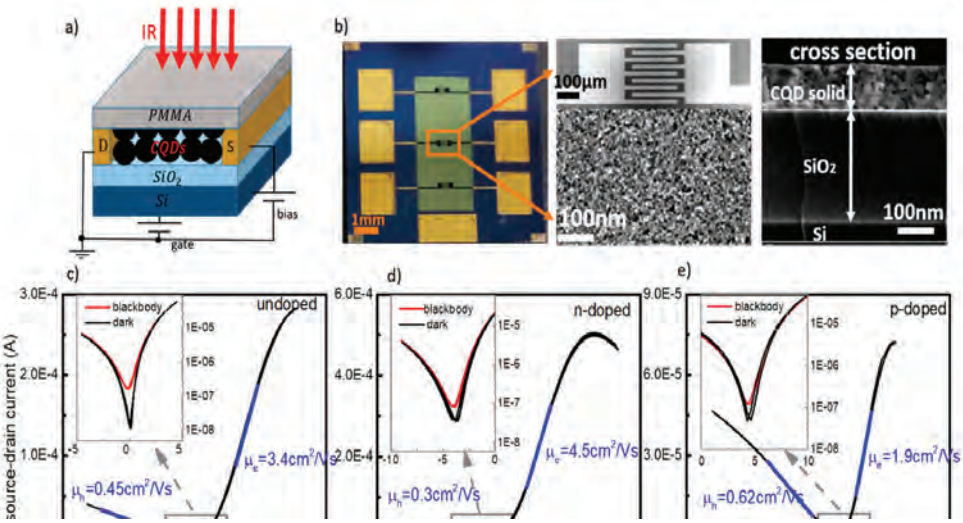

Figure 2: FET (A) schematic of a bottom-gate FET. (B) Photograph and SEM image of three FET devices of 0.3 mm x 0.16 mm. (C-E) FET transfer characteristics (at 80 K) of near-intrinsic, n-doped, and p-doped HgTe/hybrid ligand films, respectively. The insets show zoomed-in regions near the conductance minima, showing the photocurrent (red) and dark current (black). The blue lines indicate the slopes used to calculate the hole and electron mobility.

states in relation to the environmental Fermi level. This provided new insights to guide development of the best materials and processes needed to achieve high doping levels. Additionally, new techniques using excess $HgCl_2$ and a more reactive, non Hg-chelating tellurium source, Trimethylsilyltelluride produced very well dispersed HgTe colloids with a broad range of sizes. Such processes led to further development of core/shell CQDs and the highest mobility ever observed for simply drop-cast CQD films, as show in Figure 2.

Way Ahead

Work on HgS and HgSe colloidal quantum dots led to the understanding and capability to achieve core/shell quantum dots that have highly effective intersubband absorption characteristics. The HgSe core and CdS and CdSe shell based dots and thin films show much greater robustness and intense intraband luminescence that pave the way for studying their stimulated emission properties. Another aspect to this new program is the desire to quickly evaluate and transition new properties of the intersubband dot advances into focal plane demonstrations. The potential to do this was made available by a recent FY2019 DURIP award to allow such studies, but without the need for the significant follow-on efforts that were necessary to demonstrate these coherent behaviors in the past. The work provides a new foundation to establish electrically controlled and injected CQD based lasers.

Optoelectronics Program

Current Scientific Objectives

01

Explore the limits of low energy and high-speed optoelectronics to assess ways to surpass the performance of conventional electronics or consider hybrid integrated microsystems of the two, that if successful will enable much faster and higher performance computing on mobile platforms with limited power supplies

02

Advance photonics capabilities through exploration of high intensity radiation generation within microscale systems, that if successful will enable chip-scale photonic light sources from UV to mid-infrared based upon novel materials, diffractive optical techniques for beam combining, shaping, and active control for use in Army surveillance, sensing, and communications

03

Demonstrate new power scaling methods and architectures along with adaptive optical control techniques to create directed energy solutions that if successful will reduce the size and power consumption of laser systems while revolutionizing beam control performance to mitigate the effects of atmospheric turbulence for greater power delivery

Program Manager

Dr. Michael Gerhold

Program Manager, Optoelectronics

Program Manager (Acting), Electronics Sensing

Electronics Division

ARO Engineering Sciences Directorate

Dr. Gerhold completed his undergraduate studies at Purdue University, receiving his B.S. in Electrical Engineering in 1992, as well as a M.S. in Electrical Engineering in 1994. He received his Ph.D. in Electrical Engineering from the University of Michigan in 1999. He came to ARO in 1999 as the Program Manager for Optoelectronics.

SUCCESS STORY

Oxide-Free Vertical Cavity Surface Emitting Lasers Demonstrate Superior Thermal Performance

A laser of superior power and thermal performance is transitioning to industry to enable the potential development of next-generation optical interconnects, such as fiber optics for communication or electronic systems with faster response times.

Challenge

Semiconductor diode lasers have experienced success in both their edge-emitting and vertical cavity surface emitting laser (VCSEL) regimes. However, VCSELs have experienced road-blocks to achieving complete dominance of the market due to the thermal bottleneck within their active region. This bottleneck is a thermally insulating oxide which acts to control current flow into the light emitting region. However, it also causes significant increase in heat that grows as the aperture size is reduced. The future development of faster and higher-performing lasers will require discoveries that overcome this bottleneck by removing this oxide while maintaining a small-diameter beam.

Action

Beginning in 2011, the ARO Optoelectronics program manager, Dr. Mike Gerhold, identified Army-relevant research interests by Professor Dennis Deppe of the University of Central Florida's Center for Research in Electro-Optics and Lasers (CREOL). Professor Deppe is credited as the inventor of the oxide-aperture VCSEL but at that time was investigating a new approach to remove the oxide. Although Professor Deppe took great care at that time to ensure the security of his invention, Dr. Gerhold was able to gain insight into the discovery thru meaningful site visits and discussions. This interchange built upon Professor Deppe's previous relationship with both Dr. Gerhold and CCDC ARL SEDD thru DARPA and CCDC ARL programs where Professor Deppe had pursued advances for his commercially successful oxide-aperture VCSELs. The key scientific challenge at the time was the unknown mechanism of action for the new oxide-free VCSELs. Knowing the history of oxide-VCSELs and the critical function that the oxide performed, the key barrier was how one could create a laser free of this oxide - having both a small beam diameter and a small divergence angle. Prior to the oxide-VCSEL invention in the 1990s, oxide-free, proton implanted VCSELs were the standard, but they were of much lower efficiency and with slower modulation speeds due to the inability to shrink the diameter while maintaining high beam quality.

Dr. Gerhold worked with an SBIR contractor, Ultracommunications, Inc., to pioneer a working group that led to the establishment of a military standard for ruggedized optical interconnects. Operation of the interconnects from -40°C to 85°C and sometimes higher (up to 120 °C) became established requirements for various environments. However, the oxide-VCSELs clearly struggled to meet specs across this temperature range. At high temperatures their performance would degrade both in terms of reliability and output power. Dr. Gerhold's persistence to realize to implement VCSEL interconnects, in coordinate with CCDC ARL SEDD, guided the push for improved lasers.

It was Professor Deppe's phase shifting mesa placed very close to the active region which supplied the lateral isolation heretofore accomplished by the oxide. Oxide-free operation was soon proven under an ARO grant from Dr. Gerhold's program in 2012, and it quickly began to exceed expectations. The oxide-free active region was monumentally better performing than the oxide version. With just 1 micron diameter lasers, 5 mW of power could be emitted at up to 85°C or higher. Such power levels were unheard of and led Professor Deppe to immediately consider them for two important directions: integrated photonics, including silicon photonics, and for VCSEL arrays. Two patents were obtained for these applications which are yet poised for pursuit in recently announced and forthcoming programs.

This success supports these ARL Core Technical Competencies:

Network and Information Sciences

Materials and Manufacturing Sciences

This success was made possible by the following ARO S&Es or Program Specialists:

- Dr. Michael Gerhold, ARO Electronics Division

Results

- ARO established a successful collaboration between leading researchers in optoelectronics that discovered how to create a specialized laser that operates at a wider-temperature range and higher speed.
- The resulting specialized laser transitioned to IARPA to explore potential quantum computing applications.

Motivated by the challenge of developing oxide-free VCSELs into better high-speed lasers, Dr. Gerhold leveraged investments he had made with Professor Milton Feng of the University of Illinois, who was studying other high-speed optoelectronics. His group was renowned for high-speed electronics, having been the first to achieve THz speed transistors. Dr. Gerhold had invested several DURIP equipment grants for his lab, so he realized that Professor Feng could provide the needed VCSEL characterization. By organizing several years of GOMACTech technical sessions, Dr. Gerhold brought together Professors Feng and Deppe to hear about each other's work, and to consider the suggestion that they work together. As a result, each group submitted proposals that included cross-collaboration.

Result

Figure 1 shows some data from prior ARO funded research proving the viability of oxide-free VCSELs for high-speed operation across a wide military relevant temperature range. As a result of this progress on both the direct current and high-speed modulation performance of the lasers, Dr. Gerhold was able to consider some technology transition plans, which ultimately led to a new collaboration with C5ISR Center's Night Vision Laboratory (NVESD) and sdPhotonics (led by Professor Deppe), to pursue the use of cryogenic VCSELs for high-speed focal plane read-out. Professor Deppe teamed with Ultra-communications who had made great progress on two prior ARO SBIR and STTR programs in making miniaturized, low cost optical transceivers that proved to be rugged enough for any military platform.

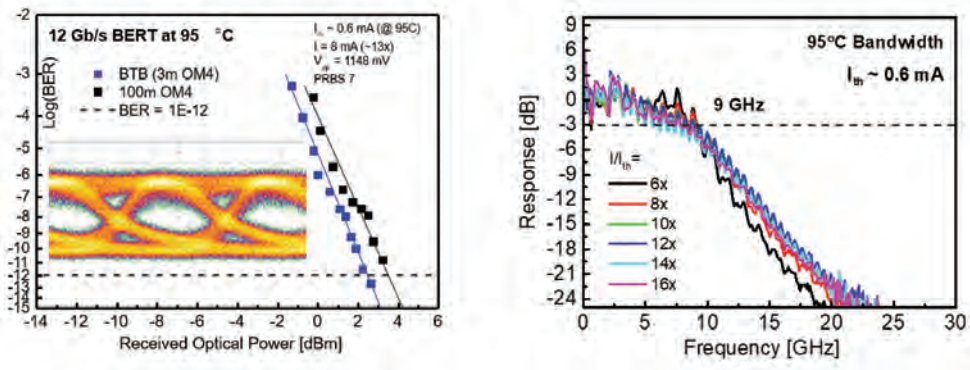

Figure 1: left) Bias dependent modulation results measured at 95 C showing 9 GHz operation; (right) Bit-Error-Rate Testing (BERT) transmission measured at 95 C showing 12 Gb/s data rate.

An additional interesting discovery, shown in Figure 2, was that the VCSELs can work well even at 4K, well below the carrier freeze-out temperature predicted in semiconductor doping theory. This led to sdPhotonics (jointly with Professor Feng) receiving a contract from a joint ARO and Intelligence Advanced Research Projects Activity (IARPA) program called "Supercables" aimed at low energy optical interconnects for superconducting qubit readout. Part of the motivation for this award is that the VCSEL threshold current exponentially decreases with temperature making them extremely efficient at 4 K, down to only tens of attojoules of energy/bit.

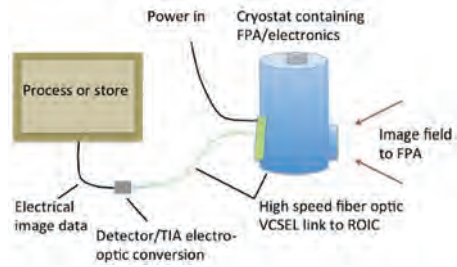

Figure 2: Cryogenic VCSEL SBIR program illustration

Way Ahead

The future of the oxide-free VCSELs is bright, especially for military applications but also for commercial endeavors. Professor Deppe recently resigned from his distinguished professorship at the U. Central Florida to focus at sdPhotonics. There he is partnering with Intelligent Epitaxial Technologies (IET) to develop a foundry supply of epitaxy for the new oxide-free VCSELs. Oxide-free VCSELs can be made smaller and more closely packed to create higher intensity beams. These results promise a new means to address high power laser systems that can couple the dense laser arrays into high brightness, high power laser beams. These high power laser systems have applications in Light Detection and Ranging (LIDAR), surveillance, and directed energy.

A new program (DARPA LUMOS) has been announced aimed at manufacturable solutions to incorporate high performing III-V compound semiconductor devices into silicon photonics foundry processes. VCSELs such as the oxide-free one of Professor Deppe are poised to be used for such studies and hold numerous potential benefits to future photonic circuit technologies. Patented approaches achieved under ARO investment provide a new foundation for much more efficient and versatile photonic systems.

SUCCESS STORY

From Slow-Light Laser to Enhanced Autonomous Navigation

ARO funded research is expected to foster the **transition of a narrow linewidth laser** to industry for the potential development of autonomous navigation systems.

Challenge

The amplitude of light is commonly used in LIDAR for range finding and in binary digital communications to indicate the two states of “1” or “0”. However, utilization of the phase of light brings much greater utility for the laser signal by providing additional information that can be garnered by creating multi-level phase states delineated in proportion to how low one can decrease the phase noise. The phase noise is directly related to the laser linewidth. Applications for both in enhanced data communications bandwidths and higher resolution LIDAR that utilizes both the amplitude and phase of the light are critical to significant system level performance advances.

Action

Narrow linewidth diode lasers known as distributed feedback (or DFB) lasers were developed by Professor Amnon Yariv of California Institute of Technology in the 1970s. They were advanced devices in their time utilizing special interference lithography techniques used to fabricate precise mirrors to create single frequency lasers with linewidths of several hundred kHz. Improving upon them became the challenge Dr. Gerhold put forth to Professor Yariv upon meeting him at ARO for the first time 2009.

This success supports these ARL Core Technical Competencies:

Network and Information Sciences

Materials and Manufacturing Sciences

This success was made possible by the following ARO S&Es or Program Specialists:

- Dr. Michael Gerhold, ARO Electronics Division

When Yariv arrived at ARO, the context had been to explore discussion of improving upon another laser pioneer's invention of the hybrid III-V/silicon laser (i.e., Professor John Bowers of the University of California at Santa Barbara) which had attracted the interest of both HP Laboratories and Intel Corporation. However, Dr. Gerhold encouraged Professor Yariv to do more than compete with Professor Bower's achievements – he asked Yariv to re-envision the potential of ultra-narrow linewidth lasers by exploring a "slow light laser." In related discussions, Professor Yariv had expressed concerns due to the difficulty of achieving repeatable, high-precision lithographic placement, but he accepted Dr. Gerhold's challenge nonetheless. After considering Dr. Gerhold's challenge further, he proposed a new laser cavity approached inspired by the DFB laser, but it incorporated slow-light designs that carefully harnessed the single frequency regime but with greater spatial control to improve coherence.

This first grant began in 2010, and Professor Yariv recruited two of the top students in the world for the work. The new approach to slow-light resonators was quickly shown to be on track. Silicon was being used as the resonator because it can be etched to have much lower waveguide loss compared to the III-V compound semiconductor gain media (InGaAsP). Studies proceeded on several fronts including the size and placement of the holes and the thickness of the critical dielectric used to bond the two parts of the laser together. This new hybrid laser that was formed resulted in amazing advances in laser linewidth from the several hundred kilohertz of established DFB lasers down to sub-kHz levels. Figure 3 shows both the cross-section (a) and top view (b) of the slow-light laser. The lower plots show the effect of changing the thickness on the spontaneous emission rate, which in turn affects the laser linewidth.

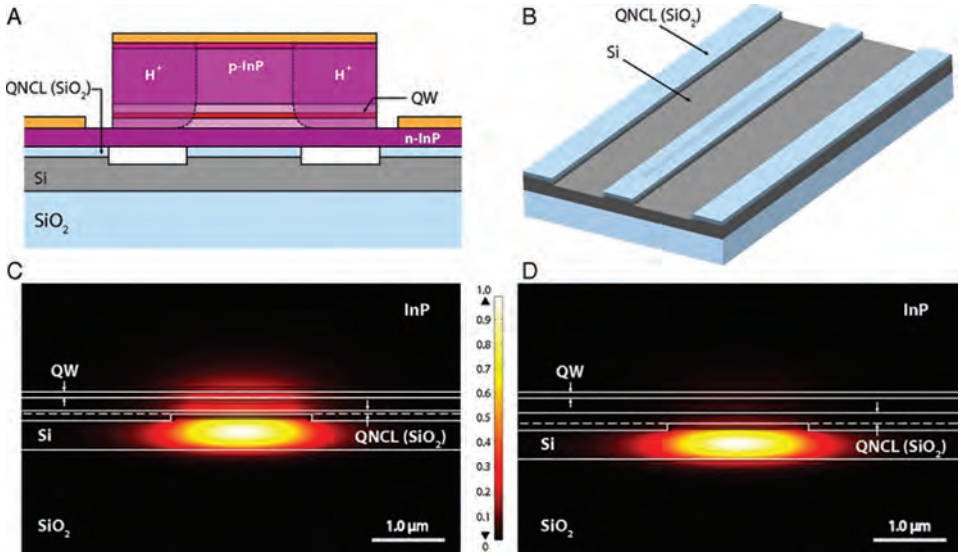

Figure 3: Spontaneous emission control on Si/III-V platform. (A) Cross-sectional structure of a Si/III-V laser featuring a SiO2, quantum noise control, spacer layer (QNCL) between Si and III-V for the modal control of the spontaneous emission rate into the laser mode. (B) A 3D schematic of the optical resonator (III-V omitted for clarity). Note that the design of the resonator accounts for the presence of the III-V (i.e., hybrid resonator). (c and d) Simulated examples of the spatial (2D) distribution of the (normalized) amplitude of the electric field (|E(r)|) of the laser mode (TE0) for two extreme cases of QNCL thickness, 50 nm (C) and 200 nm (D), representing a more than an order-of-magnitude swing in the rate of spontaneous emission. (Figure from C. T. Santis et al, "Quantum control of phase fluctuations in semiconductor lasers", PNAS, 2018)

The work continued for several years and Dr. Gerhold began to communicate the results to a number of scientists at CCDC ARL SEDD and AFRL via coordinated site visits. Others were made aware of the work through a 2015 IEEE Summer Topical meeting Dr. Gerhold organized where he invited Dr. Naresh Satyan, now the co-lead of a spin-off company from the effort, to speak. There he explained how the ultra-narrow linewidths were obtained with the same footprint as other telecommunications grade lasers, and as a result, they could produce multi-terabit per second signals from a single laser. Using

advanced control of the amplitude and phase of the laser, the implications for future data communications applications were seen as vast and led Dr. Gerhold to author an STTR topic where Telaris, Inc., the group's spin-off company, proceeded on the technology development work needed to commercialize the laser.

This STTR work delved heavily into the effect of varying a number dimensional parameters upon the resulting linewidth of the laser with the goal being to maximize the yield of the narrow linewidth lasers across the wafer. Along the way, a parallel thrust began to be pursued which became so intensive that it motivated a second phase II SBIR, in addition to the STTR. The study was upon the feedback insensitivity of the laser. Simulations of the laser proceeded with the assumption that an external optical isolator would be necessary to protect the performance of the laser from reflections. However, it became clear that the slow-light, high Q laser resonators are highly insensitive to feedback (Q means quality factor and relates to the number of times a photon is reflected within the microcavity resonator, and in this case is over a million). For economic reasons this is highly significant because in commonly used optical communications transmitters, the isolator is 5 times the cost of the laser.

Result

The result of the two phase II programs was a successful development of an ultra-narrow linewidth laser process that worked without the need for an optical isolator to be packaged with it. Furthermore, the near-kHz linewidth hybrid III-V/Si laser caused the researchers to question whether it also was suitable for LIDAR. The Intel Corporation, building upon their prior relationship with Professor Yariv and his ongoing interest in the transition of Professor Bowers' hybrid laser, saw the outstanding advances Professor Yariv had achieved beyond the more basic hybrid laser and their applicability to the autonomous navigation market. The interaction led to Telaris, Inc. being purchased by Intel to form the first ever engineering site of Intel in the city of Los Angeles. This transition is well positioned for future driver-assisted automobiles based upon coherent LIDAR – a far better prospect than amplitude only based LIDAR pursued to date. This III-V/Si ultra-narrow linewidth slow-light laser research is now poised for a solid market impact for both automobiles and military vehicles.

Way Ahead

Dr. Gerhold has continued basic research investments to explore the ultimate limits of ultra-narrow linewidth semiconductor lasers. The goal is to explore the light within a single laser resonator of similar scale to a typical DFB laser (several mm's long with single transverse mode confinement laterally). However, with this new program the concept has shifted in two major ways: (i) it leverages advances in silicon nitride based waveguides which have been engineered to far surpass the cavity Q obtainable in pure silicon, and (ii) it re-envisions the current injection thru a lateral injection scheme. Concurrently, and in coordination with Dr. Gerhold, DARPA MTO is now seeking to demonstrate the multi-Tb/s potential of the lasers. The ultra-high coherence 3-D silicon nitride/III-V semiconductor paradigm is therefore poised to revolutionize signal processing and high bandwidth communications systems well into the future.

Results

- Discovery of new slow-light distributed feedback laser with 100-1000x linewidth reduction relative to current state of the art
- New laser is expected to provide greater precision and efficiency for use in navigation and targeting via Light Detection and Ranging (LIDAR) systems
- Demonstrated rapid wafer-scale manufacturing process that will transition through the ARO STTR program for further manufacture and testing of the laser

Solid-State Electronics and Electromagnetics Program

Current Scientific Objectives

01

Discover and create unique electromagnetic phenomena in solid-state materials and structures that require theoretical formulations beyond well-established Maxwell's equations, that if achieved may enable new high frequency electronic circuits and antennas

02

Create novel device concepts with new functionality and unprecedented performance based on emerging phenomena in heterostructures and interfaces of engineered quantum materials, that if achieved may enable new electron devices with low power consumption

03

Develop novel electromagnetic structures to enable strong coupling with terahertz radiation (0.1-1 THz) and to achieve efficient generation, manipulation, and detection of the aforementioned spectral range for potential future application in high-data-rate communications

Program Manager

Dr. Joe Qiu

Program Manager, Solid-State Electronics and Electromagnetics
Electronics Division
ARO Engineering Sciences Directorate

Dr. Qiu completed his undergraduate studies at the State University of New York at Stony Brook, receiving his B.S. in Physics in 1991. He also trained as a Physicist at the State University of New York at Stony Brook, receiving his Ph.D. in Physics in 1997. He came to ARL in 2008 as an Electronics Engineer and then to ARO in 2013 as the Program Manager for Solid-State Electronics and Electromagnetics.

SUCCESS STORY

Specialized Materials for Next-Generation Integrated Circuits

This ARO initiative resulted in the **development of specialized materials** that could pave the way for what would be the **first 2D material to enter the mainstream semiconductor industry**, thereby providing a critical component technology for future generations of integrated circuits.

Challenge

Complementary metal-oxide-semiconductor (CMOS)-based integrated circuits use metal interconnect wires, which are made of aluminum and, more recently, copper, to provide electrical connections between the various circuit components. As technology node scaling has continued to fit more devices per square inch of silicon, interconnect wire cross-sections have needed to shrink, leading to increased resistivity, heating and electromigration issues. Recent investigations into the use of metals with higher melting points than copper, such as cobalt and ruthenium, have shown promising electromigration stability results, but their higher resistivities may limit their application to short local interconnects only. Similarly, attempts to use highly conductive graphene have so far been limited due to the need for high processing temperatures, which are incompatible with CMOS technologies.

Action

After a decade-long quest to achieve graphene interconnects, Professor Kaustav Banerjee and colleagues at the University of California, Santa Barbara, funded by the Army Research Office, have now developed an approach to fabricate intercalation-doped graphene nanoribbon interconnects within the thermal constraints of CMOS technology processing. Professor Banerjee first proposed the idea of using doped multi-layer graphene at the IEDM conference in 2008 and has been working on developing pieces of it, under the support and guidance of Solid-State Electronics and Electromagnetics program manager Dr. Joe Qiu. A paper describing the novel process was selected as one of the top papers from more than 230 accepted for oral presentations at the 2018 IEEE International Electron Devices Meeting (IEDM), and was one of only two papers included in the first annual "IEDM Highlights" section of the December 2018 issue of the journal *Nature Electronics*. This research could pave the way for what would be the first 2D material to enter the mainstream semiconductor industry. It is also the result of strategic collaboration between Dr. Qiu and Materials Science Division at ARO to enable novel device concepts through material discoveries. ARO has been at the forefront of 2D material discoveries for the past 10 years.

Result

In February 2017, Professor Banerjee demonstrated the first Chemical Vapor Deposition (CVD) of multilayer graphene at a high temperature, subsequently transferring it to a silicon chip, and then patterning the multilayer graphene, followed by doping.

This success supports these ARL Core Technical Competencies:

Materials and Manufacturing Sciences

Computational Sciences

This success was made possible by the following ARO S&Es or Program Specialists:

- Dr. Joe Qiu, ARO Electronics Division
- Dr. Chakrapani "Pani" Varanasi, ARO Materials Science Division

Results

- Selected as one of the top papers from more than 230 accepted for oral presentations at the 2018 IEEE International Electron Devices Meeting (IEDM), which is world's preeminent meeting for electron devices technology
- One of only two papers included in the first annual "IEDM Highlights" section of the December 2018 issue of the prestigious journal *Nature Electronics*
- Demonstrated graphene-based interconnect technology with smallest width for use in future integrated circuits
- Demonstrated a new and unique process for synthesizing large area high quality graphene material

Electrical characterization of the conductivity of DMG interconnects down to a width of 20 nanometers established the efficiency of the idea that had been proposed in 2008. However, the process was not "CMOS-compatible" (the standard industrial-scale process for making integrated circuits), since the temperature of CVD processes far exceed the thermal budget of back-end processes. To overcome this bottleneck, Professor Banerjee's team developed a unique pressure-assisted solid-phase diffusion method for directly synthesizing a large area of high-quality multilayer graphene on a typical dielectric substrate used in the back-end CMOS process (Figure 1). Solid-phase diffusion, which is well known in the field of metallurgy and is often used to form alloys, essentially involves applying pressure and temperature to two different materials that are in close contact so that they diffuse into each other. Professor Banerjee's group employed the technique in a novel way. They began by depositing solid-phase carbon in the form of graphite powder onto a deposited layer of nickel metal of optimized thickness, then applied heat (300 degrees Celsius) and nominal pressure to the graphite powder to help break down the graphite. The high diffusivity of carbon in nickel allows it to pass rapidly through the metal film. How much carbon flows through the nickel depends on its thickness and the number of grains in it. Deposited nickel is not a single-crystal metal, but rather a polycrystalline metal, meaning that it has areas where two single-crystalline regions meet each other without being perfectly aligned. These areas are called grain boundaries, and external particles-in this case, the carbon atoms-easily diffuse through them. The carbon atoms then recombine on the other surface of the nickel closer to the dielectric substrate, forming multiple graphene layers. Professor Banerjee's team was able to control the process conditions to produce graphene of optimal thickness. The nickel thickness and other process parameters are optimized to obtain precisely the number of graphene layers at the dielectric surface. Subsequently, the nickel is removed by etching so that what's left is only very high-quality graphene-virtually the same quality as graphene grown by CVD at very high temperatures. Because the process involves relatively low temperatures, it would not damage other fabricated elements on the same substrate. CMOS-compatible doped-graphene-nanoribbon (DGNR) interconnects fabricated by subtractive etching process, with smaller resistivity than that of Cu, Co and Ru interconnects, and negligible electromigation, are demonstrated for the first time down to 20-nm width.

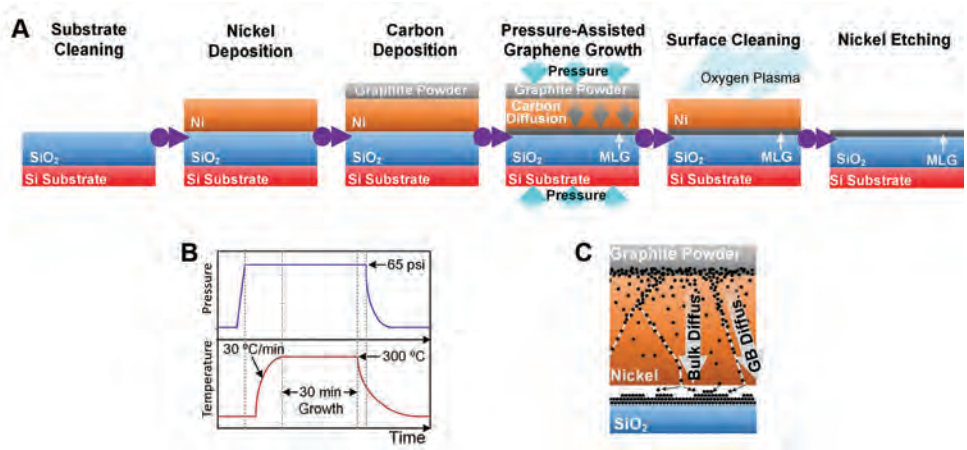

Figure 1: (A) Schematic of pressure-assisted low-temperature graphene growth. (B) Pressure and temperature profiles for the low-temperature graphene growth. (C) Schematic of the pressure-assisted graphene growth mechanism.

Way Ahead

The University of California - Santa Barbara has filed a provisional patent on the process, which overcomes the obstacles that, until now, have prevented graphene from replacing copper. Overall, graphene interconnects help to create faster, smaller, lighter, more flexible, more reliable, and more cost-effective integrated circuits. Professor Banerjee is currently in talks with industry partners interested in potentially licensing this CMOS-compatible graphene synthesis technology, which could pave the way for what would be the first 2D material to enter the mainstream semiconductor industry. The UCSB researchers will also visit CCDC ARL SEDD to establish collaborations to demonstrate prototype integrated circuits incorporating DGNR interconnects.

SUCCESS STORY

Wafer-Scalable, Aligned Carbon Nanotube Transistors Exceeding 100 GHz Frequencies

This ARO initiative resulted in the development of **carbon nanotube field-effect transistors with world record speed exceeding 100 GHz and superior linearity performance.**

Challenge

Semiconducting single-walled carbon nanotubes (CNTs) have very desirable characteristics which are ideal for field-effect transistor (FET) channels, such as one-dimensional (1D) ballistic transport, high carrier mobility, inherent linearity and small size. Such an enabling technology will have a major impact in reducing size, weight, power and cost (SWAP-C) of RF electronics. Modern wireless technology increasingly relies on highly linear devices to achieve spectral-efficient modulation (that is, more data per unit bandwidth) and high spurious-free dynamic range for extracting weak signals from increasingly crowded airwaves. Achieving high-linearity at low DC power levels would be an additional advantage for power constrained applications. However, after more than 2 decades of intense research, these potentials were not fully realized due to a number of technical challenges: 1) the lack of techniques to eliminate tube-tube cross junctions and achieve parallel aligned CNT arrays with optimal packing density of CNTs; 2) the presence of metallic CNTs leading to less than ideal semiconducting purity; 3) difficulty of creating highly conductive ohmic contact to the CNT arrays.

Action

With a vision for realizing disruptive CNT-FETs, Solid-State Electronics and Electromagnetics program manager Dr. Joe Qiu authored an innovative Small Business Technology Transfer (STTR) topic to transition university-led research results to commercial devices. Carbonics, Inc. partnered with the University of Southern California successfully developed a carbon nanotube technology that, for the first time, achieved speeds exceeding 100GHz. The milestone eclipses the performance – and efficiency – of traditional Radio Frequency Complementary Metal-Oxide Semiconductor

This success supports these ARL Core Technical Competencies:

Network and Information Sciences

Materials and Manufacturing Sciences

This success was made possible by the following ARO S&Es or Program Specialists:

- Dr. Joe Qiu, ARO Electronics Division

Results

- Research published in prestigious journal *Nature Electronics*
- First Carbon nanotube field-effect transistors with world record speed exceeding 100 GHz
- Demonstrated the only transistor technology that not only offers high performance but also provides integration compatibility with current integrated circuit fabrication process

(RF-CMOS) technology that is ubiquitous in modern consumer electronics, including cell phones. Projections based on scaling single carbon nanotube device metrics suggest the technology could ultimately far exceed the top-tier incumbent RF technology, Gallium Arsenide (GaAs). The STTR program, under the proactive leadership of Dr. Qiu, focuses on feasibility studies leading to prototype demonstration of technology for specific applications. The technology used by Carbonics also traces its origin to the work done by Professor Peter Burke's group of the University of California at Irvine, which was previously supported by the ARO Electronic division. One of Professor Burke's former graduate students, Dr. Christopher Rutherglen, is now the chief technology officer of Carbonics.

Result

Carbonics has demonstrated a wafer-scalable approach for producing aligned CNT-FETs with extrinsic fT and fmax performance distribution exceeding 100 GHz and, linearity metrics OIP3 normalized to DC power and P1dB both exceeding 10 dB. These capabilities, which challenge those of incumbent RF amplifier technology, are the result of the benefits of 1D materials – namely, reduced scattering, small parasitic capacitance, and high linearity – and were achieved through refinements in CNT deposition and device processing.

Dense, aligned arrays of high-semiconducting-purity (> 99.9% as determined optically), polymer-sorted single-walled carbon nanotubes (SWNTs) with linear densities of 40 – 60 CNTs/μm (inclusive of individual CNTs and bundles of ≥ 2 CNTs) were deposited over a 20×30 mm area of the wafers using a technique that is a modified version of the floating evaporative self-assembly process first co-developed by the Arnold and Gopalan Groups at the University of Wisconsin, Madison (Figure 2). Fabrication of the RF CNT-FET devices were performed using standard, scalable, semiconductor tools on 100 mm diameter, single-crystal quartz wafers.

After the aligned CNT deposition, a combination of electron-beam lithography (EBL) and stepper-based photolithography were used for all patterning. Source and drain contact electrodes were patterned first by EBL in order to 1) deposit the Pd contact metal onto the cleanest possible interface by avoiding accumulated contaminants from subsequent processing, 2) decouple the source-drain length dimension from that of the gate size which is a constraint when self-aligned contacts are used, and 3) to reduce the accumulation of

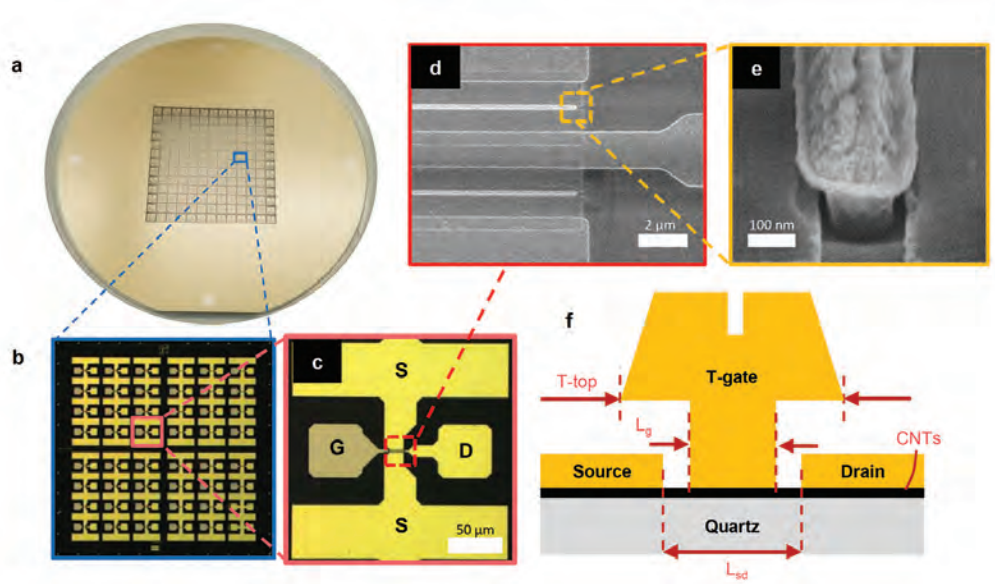

Figure 2: CNT-FET devices fabricated with a wafer-scalable process. (A) CNT-FET T-gate devices were fabricated on 100 mm quartz wafers. (B) Optical micrograph of test dies around the perimeter of the patterned dies. (C) Optical micrograph of the co-planar waveguide structure of a single CNT-FETs. (D) SEM image of one edge of CNT-FET device. (E) SEM image of a T-gate cantered in the channel. (F) Depiction of CNT-FET device cross-section.

CNT bundling during processing. This was followed by photolithographically patterning the CNT channel area and metal pads in a co-planar waveguide arrangement. The devices utilize a T-gate geometry, commonly used in III-V HEMT devices, since it is effective at minimizing the gate-length (for fast carrier transit times) while simultaneously minimizing the gate-resistance (by increasing the overall gate cross-section).

The research was published in the journal *Nature Electronics*.

Way Ahead

The results by Carbonics suggest that CNT-FET technology could ultimately offer both the high performance of GaAs pHEMTs and integration compatibility with CMOS. The next steps will be to further improve the linearity, as well as investigate noise characterization and optimization. Carbonics also has plan to collaborate with CCD ARL SEDD for more detailed device characterization utilizing ARL's unique digital waveform synthesis facilities which is capable of simulating realistic waveforms used in wireless 5G and military communications systems.

Materials Design Program

Current Scientific Objectives

01

Generate new fundamental knowledge of self-assembly by elucidating the multiple physical and chemical forces at play during directed, bottom-up 3D assembly of super-structures that incorporate multiple components that if successful, will support the deterministic design and creation of novel multi-functional materials with targeted properties, behavior, and capabilities for the next generation of Army materiel

02

Develop reconfigurable materials that can reversibly change their properties and hierarchically structured materials that display novel emergent or collective behavior that if successful, will enable advanced "smart materials" concepts like reconfigurable optics and electronics, dynamic camouflage, and adaptive sensors

03

Leverage recent advances in machine learning, artificial intelligence, data science, and other numerical approaches to solve difficult and complex materials design problems related to self-assembly and reconfigurability that if successful, will enable data-driven, inverse design of advanced materials starting from desired properties and functionality, as well as novel models, algorithms, and experimental approaches to designing stronger, lighter weight, and adaptive structural or protective materials for the Soldier

Engineering Sciences Directoriate

- Electronics Division
- **Material Sciences Division**
- Mechanical Sciences Division

Program Manager

Dr. Evan Runnerstrom
Program Manager, Materials Design
Materials Science Division
ARO Engineering Sciences Directorate

Dr. Runnerstrom completed his undergraduate studies at Stanford University, receiving his B.S. in Materials Science and Engineering in 2009. He trained as a Materials Scientist at the University of California, Berkeley, receiving his Ph.D. in Materials Science and Engineering in 2016. He came to ARO in 2019 as the Program Manager for the Materials Design Program.

SUCCESS STORY

Self-Assembling Soft Matter at Liquid Interfaces

ARO has established **high-impact research activity on self-assembly at liquid surfaces and interfaces**, leading to new soft materials that will impact future Army-relevant technologies like micro-robotics, water harvesting and purification, and reconfigurable optics.

This success supports these ARL Core Technical Competencies:

Protection Sciences

Materials and Manufacturing Sciences

This success was made possible by the following ARO S&Es or Program Specialists:

- Dr. John Prater (retired), ARO Materials Science Division
- Dr. Evan Runnerstrom, ARO Materials Science Division

Challenge

Understanding how colloids and polymers assemble at liquid-liquid and liquid-solid interfaces is critical to designing materials capable of directed 3D self-assembly, and is rapidly becoming a keystone topic in colloid and surface science. Liquid-phase phenomena and particle assembly at liquid interfaces in both hard and soft materials have long been recognized as critically important to mature technologies like ore extraction and emulsion stabilization. Contemporary research has emphasized the use of surfactants, polymers, and colloids to create stable, multi-component 3D structures in the liquid phase. Despite these efforts, achieving arbitrary 3D shapes and dynamic behavior has been challenging. Most self-assembled structures based on liquid interfaces adopt equilibrium spherical shapes to minimize interfacial area, complicating the route to generating more complex functional structures. Additionally, these assemblies typically adopt a local thermodynamic equilibrium that resists the external forces needed for reconfigurability.

Action

In the year 2011, the Materials Design Program Manager, Dr. John Prater launched a new “reconfigurable materials” thrust, with the goal of developing the expertise needed to design and fabricate robust multi-functional materials. During this time, Dr. Prater organized a Special Topics Workshop on Self-Assembly (September 2011) and co-organized the 2015 ARL Army Science Planning and Strategy Workshop on Microscale Adaptability (with ARO PMs Dr. Dawanne Poree and Dr. David Stepp). Dr. Prater’s vision in this area has enabled the Army’s basic research program to identify and advance a number of important areas, including:

1. Combination of self-assembly techniques and 3D printing to achieve hierarchical nano-constructs, which provide a viable pathway to developing "living materials."

2. Studies of cephalopod-based (i.e., cuttlefish, squid, octopus) natural adaptive camouflage and developing materials to mimic this process.

3. Computational techniques to streamline the development of new materials, including emerging concepts of reconfigurable meta-materials with radically new capabilities (e.g., cloaking).

Recognizing a particular opportunity for scientific advances in self-assembly at liquid interfaces, Dr. Prater invited single-investigator proposals from two renowned scientists, Professor Thomas Russell of the University of Massachusetts at Amherst and Professor Kathleen Stebe of the University of Pennsylvania. These projects, titled "Liquid Tubules by the Self-Assembly of Self-Regulating Nanoparticle Surfactants" and "Curvature Directed Assembly of Particles into Reconfigurable Structures at Fluid Interfaces", respectively, began in 2016 and continued through 2019 under the management of Dr. Evan Runnerstrom, who took over the Materials Design program upon Dr. Prater's retirement. Dr. Runnerstrom continued to support these research activities, and also facilitated a new academic-Army cooperative agreement, titled "Soft, reconfigurable photonic systems inspired by cephalopod chromatophores: A platform to study dispersed light sensing in squid." This collaboration is between Professor Leila Deravi of Northeastern University, Professor Daeyeon Lee of the University of Pennsylvania, and Dr. Richard Osgood of CCDC SC.

Result

Over the course of their ARO-supported projects, both Professors Russell and Stebe have made remarkable discoveries related to liquid interface self-assembly and reconfigurability. A strong collaboration has already been established between CCDC's Dr. Osgood and Professors Deravi and Lee; they are working to develop artificial liquid-phase self-assembled materials that can mimic the natural camouflage mechanisms of squid and octopus. These projects supported five graduate students and two postdoctoral research scholars. Below are highlighted two particular research achievements: structured water-in-water systems that mimic living cells (Russell), and autonomous motion of colloidal particles within liquid crystals (Stebe).

Professor Russell has spearheaded the development of charged polymer (polycations, polyanions) interactions at water/water interfaces to generate kinetically trapped, all-liquid structures of non-equilibrium shapes. These shapes can be designed to achieve new, targeted functionality, such as bio-mimicry. Biological systems are notable for their ability to compartmentalize and coordinate system functions in all-water-based systems, which has been difficult to reproduce in synthetic systems. Using their all-liquid structures, Professor Russell's research group has demonstrated a novel strategy to fabricate 3D compartmentalized water-in-water constructs, stabilized by a polyanion-polycation membrane. These structures are also amenable to 3D printing, which allows for precise control over their length, shape, and feature size. These all-aqueous printed structures provide a unique platform for the study and fabrication of more controlled, complex, and even compartmentalized all-aqueous systems. Such all-aqueous systems support continuous selective diffusion across the membranes and compartmentalized chemical reactions; the Russell group has developed systems where two complex

chemical reactions can occur simultaneously but in separate compartments, which allows the products of one reaction to selectively diffuse across the membrane to drive a reaction in the second compartment. This work culminated in a 2019 publication in the high-profile journal *Chem* (Figure 1). This was accompanied by media attention and a press release that quoted both Professor Russell and Dr. Runnerstrom (https://www.arl.army.mil/www/default.cfm?article=3490).

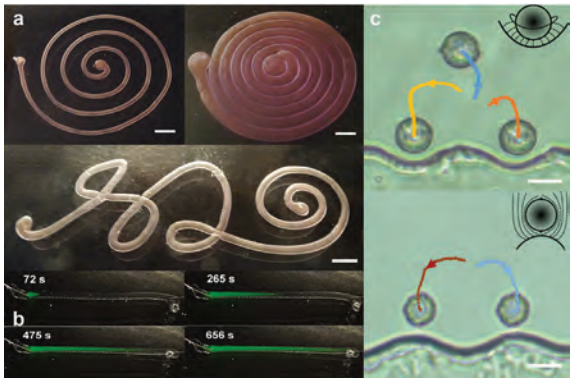

Figure 1: a: Example of 3D-printed water-in-water structures created by Professor Russell's group. b: Time-lapsed images showing transport of fluorescent solution through a 3D-printed water-in-water tube, mimicking the biological transport processes in living systems. [G. Xie, et al., *Chem*, 5 (2019), 2678-2690.] c: Composite images showing tunable trajectories of colloidal particles moving in a liquid crystal in proximity to a curved interface (Professor Stebe's group). The inset illustrations depict the nature of the liquid crystal deformations induced by the colloid, which dictates colloid motion near the wavy wall. [Y. Luo, et al., *Nature Communications*, 9 (2018), 3841.]

Professor Stebe has pioneered the use of liquid crystals to influence and direct colloidal self-assembly. Colloidal assembly is widely employed to efficiently build hierarchically ordered structures, but the ability to precisely dictate colloid dynamics, equilibrium states, and reconfiguration of colloidal structures has been elusive. Liquid crystals are a potential solution, as they have a dual nature that makes them ideally suited for reconfigurable colloids. As fluids, they provide an environment in which colloids can move. As crystals, they store elastic energy when distorted from an aligned and uniform orientation. Colloids placed within liquid crystals cause local distortions that can be tuned by shape and surface chemistry. These local distortions lead to colloid motion, which can be used to direct colloid assembly along paths than can be defined by curved "wavy" walls. By placing magnetic colloids using an external magnetic field at particular locations, and releasing that field, colloids are autonomously propelled on well-defined trajectories. Reversibility is easily achieved by re-applying the external field. Notably, these interactions do not depend on the particular material used for the colloid or the wavy wall, so these schemes can be exploited to build structures from diverse materials. Professor Stebe and the Penn Center for Innovation are pursuing a patent for this work.

Way Ahead

Professor Stebe's research group will move next to controlling colloid motion and reconfigurability in higher dimensions and in more complex environments. Success may pave the way for reconfigurable optical metamaterials and micro-robotic functionality. Professor Russell's research group plans to extend their studies on water-in-water interfaces and structures to functional structures and devices that could be used for chemical separations, sensing, or energy storage. Success here may lead to designed self-assembled structures that can be used to isolate or stabilize chemical reactions in a bio-compatible all-water environment, with the potential for researchers to design new materials for water purification, water-based batteries, and drug delivery. With an eye towards potential technology transition opportunities for the Army, Dr. Runnerstrom has briefed this work to ARL leadership and will continue to engage CCDC SC scientists working on Soldier-level power and water production. Dr. Runnerstrom will continue to closely follow the collaboration between CCDC SC and Professors Deravi and Lee as they work to study the fundamental materials science associated with artificial adaptive camouflage.

Results

- Five high-impact publications from ARO-supported researchers studying self-assembly at liquid interfaces
- Three patent applications filed by ARO-supported researchers in this area
- Self-assembled water-in-water structures (Professor Russell) and other related single-investigator grant results briefed to interested CCDC SC scientists
- Cooperative agreement established between Northeastern University, The University of Pennsylvania, and the CCDC Soldier Center to study and mimic biological camouflage mechanisms
- Professor Thomas Russell elected to National Academy of Inventors

SUCCESS STORY

Designing Materials That Respond to Their Environment

ARO workshop and funding initiatives **established a new scientific field** that integrates self-assembly, responsive materials, and additive manufacturing to **design and create synthetic "living" materials systems** that can autonomously translate environmental stimuli into meaningful action.

Challenge

The future Army will require dynamic, responsive, and multi-functional materials that sense, react to, and report on changes to their environment. Living biological systems display exquisite ability to translate environmental stimuli into meaningful actions, and they can do so autonomously. There are currently no synthetic materials systems that do this. Addressing this need is challenging because most materials are optimized for a single, specialized purpose, which limits their functionality and adaptability. Designing multi-functional materials that autonomously react to their environment requires a paradigm shift in the materials design approach, along with sustained, multi-disciplinary effort.

Action

In 2015, Dr. Prater and ARO Chemical Sciences PM Dr. Dawanne Poree identified a significant research opportunity in integrating responsive materials with emerging additive manufacturing approaches. Dr. Prater, Dr. Poree, and ARO Materials Science PM Dr. David Stepp co-organized a workshop on this topic for the 2015 ARL Army Science Planning and Strategy Meeting. The workshop, titled Microscale Adaptability, explored how novel molecular building blocks could be integrated with novel assembly and processing techniques to design and create new materials with unprecedented responsive and reconfigurable properties. Conclusions from the workshop, published in the 2015 Army Science Planning and Strategy Report, identified three research areas—Self-Assembly of Reconfigurable Elements, Responsive Behavior, and Engineered Interfaces—that warranted sustained multidisciplinary exploration to enable significant advances for the future Army.

Seeing that a MURI-scale program was an ideal vehicle to begin addressing this challenge, Dr. Prater and Dr. Poree co-authored a FY17 MURI topic titled "Additive 3D Self-Assembly of Responsive Materials". The topic was developed with extensive input from DoD scientists and program managers at ARL, ARO, NRL, ONR, AFRL, AFOSR, CCDC SC, and DARPA. They challenged the scientific community to push beyond the existing self-assembly paradigms to create dynamically responsive, hierarchically ordered systems that integrate multiple complex functional materials and properties.

Result

The winning proposal in response to this MURI call came from a notable multidisciplinary and high-impact team led by Professor Anna Balazs of the University of Pittsburgh. Her team's overarching objective is to create synthetic materials systems that, just like living systems, seamlessly incorporate an artificial "musculoskeletal

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Protection Sciences

Materials and Manufacturing Sciences

This success was made possible by the following ARO S&Es or Program Specialists:

- Dr. Dawanne Poree, ARO Chemical Sciences Division
- Dr. John Prater (retired), ARO Materials Science Division
- Dr. David Stepp, ARO Materials Science Division
- Dr. Evan Runnerstrom, ARO Materials Science Division

Results

- High-impact multidisciplinary project with multiple-PI team formed to create multi-functional materials that sense, react to, and report changes in their environment
- 17 journal papers in high-impact journals published or in press thus far by the multidisciplinary research team
- Established academic-Army collaborations with anticipated future transitions to ARL, the Air Force Research Laboratory, and the CCDC Soldier Center

system", "nervous system", and a "metabolism" to perform multiple functions in response to their environment. To do so, they are developing the basic experimental and theoretical approaches to integrate materials synthesis, microscopic self-organization motifs, characterization, and 3D printing to create a new class hierarchical materials with integrated "bones", "muscles", "nerves", sensors, and internal energy generation. A strong theory and simulation component to this research provides fundamental insight into the behavior of individual components as well as the integrated systems.

The ultimate goal is the design of "smart" materials that can self-regulate, morph, camouflage, harvest and store energy, and display dynamic adaptive behavior in multiple environments. In pursuit of this goal, the MURI team is exploring three discrete thrusts:

1. Self-assembly of microscale musculoskeletal frameworks.
2. Transducing mechanical, chemical, electrical, and optical energy into physical functions.
3. 3D printing of large-scale adaptive materials.

The team enjoyed a number of notable achievements in these three areas in 2019 (Year 3 of the MURI grant). A particularly remarkable result appeared in *The Proceedings of the National Academy of Sciences* in 2019, in which the MURI team introduced stimuli-responsive microstructures based on liquid-crystalline elastomers (LCEs), a class of material that combines the functionality of polymers and liquid crystals. These LCEs could be polymerized in the presence of a magnetic field, which allowed for encoding specific motion responses into the LCE microstructures (e.g., twisting, tilting, stretching) at the liquid crystal nematic-isotropic transition temperature. The team was

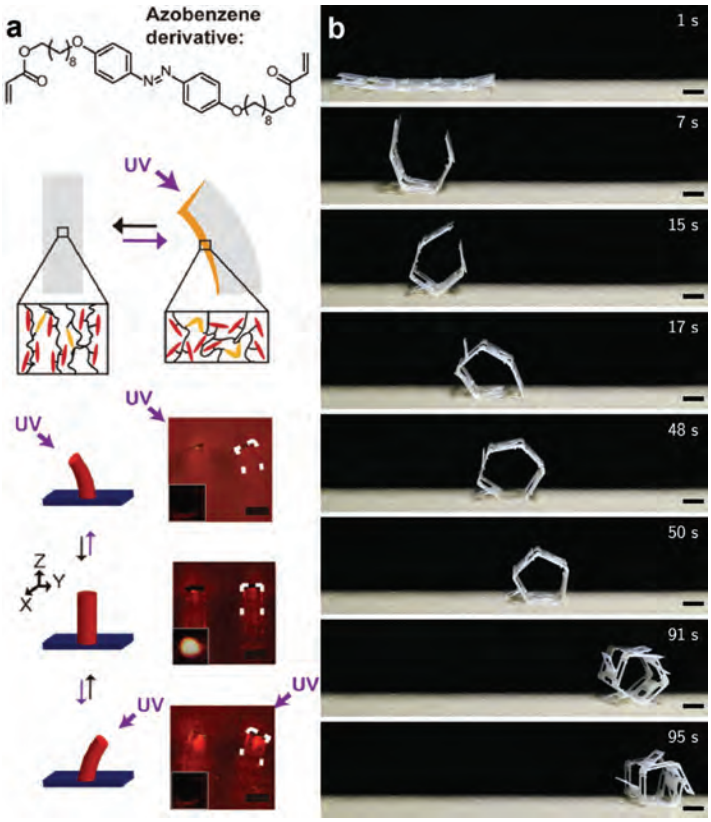

Figure 2: A: Light-responsive actuators based on liquid-crystalline elastomers (LCEs). The patterned LCE posts autonomously respond to UV light. [Y. Yao, et al. *PNAS*, 51 (2018), 12950-12955.] B: 3D printed soft "roll-bots" are capable of autonomous self-propulsion on a heated surface. [A. Kotikian, et al. *Science Robotics*, 4 (2019).]

additionally able to incorporate light-sensitive components within the LCEs to achieve greater multi-functionality through light-actuated motion. Patterned LCE microstructure arrays can exploit this responsive multi-functionality to release cargo, camouflage, and control reflectivity. This type of programmable behavior will likely form a critical foundation for autonomous and responsive smart materials. Other prominent MURI team accomplishments in 2019 include 3-D printed soft robots ("roll-bots") capable of self-propulsion on a heated surface (*Science Robotics*), and engineered wide-angle, spectrally selective light absorption and emission in inverse-opal structures (*ACS Photonics*).

Way Ahead

Dr. Runnerstrom took over management of this effort from Dr. Prater upon his retirement, with Dr. Poree continuing to co-manage the effort. The MURI team is poised to become a major innovator in the fields of self-assembly and reconfigurable matter. Building on the fundamental advances described above, their focus going forward is design integrated, hierarchical objects that seamlessly incorporate multiple the functions necessary to perform spatially and temporally coordinated actions. Responsive materials that are simultaneously adaptive, flexible, lightweight and strong may help establish new paradigms for the next generation of smart sensors, self-regulating entities, active camouflage, light gathering / beam steering systems, and medical implants for patient care and diagnostics.

Recognizing this potential, the MURI team is pursuing numerous DoD collaborations in conjunction with this work, particularly with ARL WMRD, CCDC SC, and the AFRL Materials and Manufacturing Directorate. The co-PIs are additionally encouraging their eligible students to visit DoD labs. Establishing these connections will provide potential pathways for technology transition. The third-year MURI review is scheduled to take place at CCDC SC in spring 2020, based on significant interest from scientists and engineers there.

Mechanical Behavior of Materials Program

Current Scientific Objectives

01

Create, design, and optimize a broad range of robust mechanochemically adaptive materials, based on exquisite control of force-activated molecules and force-activated reactions that if successful could lead to self-reporting structural components and adaptive symbiotic fabrics for Soldier protection

02

Tailor the deformation and failure mechanisms in materials to mitigate the propagation of intense stress-waves and control energy dissipation that if successful may lead to blast reflecting materials and novel therapeutics for blast battlefield exposure to protect the Soldier

03

Establish and optimize new atomic-scale strengthening mechanisms governing bulk mechanical behavior that if successful is anticipated to lead to new lightweight protective fabrics and equipment

Program Manager

Dr. David Stepp
Program Manager, Mechanical Behavior of Materials
Materials Science Division
Director of Engineering Sciences
ARO Engineering Sciences Directorate

Dr. Stepp completed his undergraduate studies at Harvey Mudd College, receiving his B.S. in Engineering in 1993. He trained as a materials scientist at Duke University, receiving his Ph.D. in Mechanical Engineering and Materials Science in 1998. He came to ARO in 1999 as the Program Manager for Mechanical Behavior of Materials and was promoted to the Division Chief, Materials Science Division, in 2004 and then to the Director, Engineering Sciences, in 2016.

SUCCESS STORY

Motif Structures in Polymer Nanocomposites

This ARO initiative resulted in the **discovery of motif structures at the critical filler-matrix interface of polymer nanocomposites**, providing new mechanical strengthening strategies for lightweight aerospace, Soldier protection, and flexible electronic applications.

This success supports these ARL Core Technical Competencies:

Materials and Manufacturing Sciences

Computational Sciences

This success was made possible by the following ARO S&Es or Program Specialists:

- Dr. David Stepp, ARO Materials Science Division
- Dr. Dan Cole, Tech Advisor to the ARO Materials Science Division

Challenge

Considerable advances have been made in large scale production of polymer composites (e.g. Boeing 787 Dreamliner), and a wide range of laboratory-scale advanced composite materials have been demonstrated. These advances have led to a vision of future smart polymeric materials with many exciting applications, including environmentally-adaptive skins, electro-active components, structural power storage, self-healing materials, and structural sensors. The material behavior of polymer composites are governed by the interface between the matrix (i.e. polymer) and filler (e.g. relatively stiff particles or fibers, particles with excellent electrical and thermal conductivity, etc.). Specifically, these interactions are controlled by an "interphase" or the region *between* the matrix and filler. Composites with nanoscale fillers have extraordinarily high interfacial areas (10^2-10^3 m^2/g), making the interphase properties particularly important.

For over two decades now, researchers have been trying to use nanoscale fillers to enable lightweight nanocomposites with extraordinary mechanical properties. However, these mechanical gains have been mostly modest due to poor control of the interphase, preventing sufficient dispersion of the filler within the matrix, as well as poor load transfer between matrix and filler when subject to mechanical stress. Another key challenge with this advanced nanocomposite research is the lack of *mechanistic*—or physics-based—understanding of interphase interactions. Most material models assume a homogenization of properties (e.g. interphase volume, interphase mechanical properties) and do not account

for randomization. Therefore, designing an optimal material architecture, predicting material failure, or enabling new types of multifunctional material behavior has been greatly limited.

Action

This success originated from a staff research collaboration between Dr. William Mullins, the Synthesis and Processing of Materials program manager, and Professor Greg Forest at the University of North Carolina - Chapel Hill. The collaboration sought to address a key challenge in the nanocomposites community related to understanding mechanical percolation behavior (i.e. the threshold for sufficient filler-filler interactions to cause a significant increase in mechanical properties). After Dr. Mullins pursued a different position, Mechanical Behavior of Materials (MBM) program manager Dr. David Stepp encouraged Professor Forest to submit a proposal on the topic based on the unique approach he was exploring, from the applied mathematics perspective, to describe this complex material system through network graphs, a mathematical construct that considers pairwise relations between objects in a network.

Based on promising results with the network approach to describing the complex composite behavior, Dr. Stepp encouraged an enhanced multi-researcher follow-on effort incorporating an experimental project to validate the model. The results of the network approach also provided new insights on a previously unexplained phenomena Dr. Stepp had learned about under the DARPA Advanced Structural Fiber Program with Professor Satish Kumar of Georgia Tech, whereby very low fractions of carbon nanomaterials (<1% by volume) were showing some of the most significant increases in mechanical properties (i.e., far exceeding those of larger concentrations). This integrated modeling/experimental project on a specific polymer nanocomposite system led to the discovery of “motif” structures, which were crystalline regions around the filler that occurred at a specific weight percent and led to extraordinary increases in the thermomechanical behavior of the material.

Encouraged by these potentially transformative results, Dr. Stepp organized a review of Professor Forest’s team in the Fall of 2018 and invited ARO Program Manager Dr. Jim Harvey and Dr. Dan Cole, an ARL scientist serving as technical advisor to the MBM program. During the review, the group began a dialogue about various characterization techniques that could be used to further understand how the local behavior of the motifs control the overall mechanical performance of the composite. In addition, Drs. Stepp and Cole, with the help of Dr. Leah Wingard of CCDC ARL WMRD, organized an invited seminar, lab tours, and one-on-one meetings at WMRD in the Spring of 2019. Several samples transitioned to ARL for testing, and as a result, multiple co-authored journal publications between investigators and ARL researchers are in preparation.

Result

This effort tested the scientific hypothesis that mechanical percolation results when the reinforcing fillers have sufficient volume fraction that the phase may coalesce into a rigid scaffold, with the filler particles in close contact and constrained from certain types of movement. The principal investigator (PI) treated this complex material system as a network, with each filler object considered as an element able to sense and be affected by neighbors. The group identified a number of primitive rigid motifs that may serve as building blocks for larger rigid aggregates. This result was important as a step toward simulating how the composite behaves during fabrication and provides key information for tuning process parameters in order to optimize mechanical performance.

Results

- Polymer composite system for structural applications in extreme thermomechanical environments
- Advanced composites transitioned to ARL for nano/microscale mechanical testing
- Multiple co-authored journal publications between Army and academic researchers are in preparation
- Co-PI presented results at CCDC ARL through an invited talk in 2019

This initial success in developing a network science-inspired mathematical model for composites motivated a collaboration with an experimental polymer chemist. The team focused on a polyetherimide (PEI) system, which is typically an amorphous polymer at room temperature, meaning the chains have no long range order. For a filler, the team chose single wall carbon nanotubes (SWCNTs), due to the exceptional material properties and high aspect ratio, giving opportunity for each filler element to interact with many others. The PEI-SWCNT composite was a well-studied material system, but the team's approach for pursuing extraordinary mechanical behavior was unconventional. Whereas most groups were focused on mechanical load transfer from matrix to filler (and hindered by the processing challenges mentioned previously), the team instead used the nanofiller template to confine the interphase and induce stiffness through the polymer itself.

The resulting research created a feedback loop between modeling and experimental efforts, providing key information on both ends. This eventually led to the discovery of a "motif" material structure in the PEI-SWCNT composites, essentially a crystalline interphase growth seeded at the surface of the SWCNT filler. This structure was responsible for significant gains in thermomechanical performance with an extremely low concentration of the filler (approximately 0.1% by volume). The group established a collaboration with Oak Ridge National Laboratory (ORNL) and used a technique known as small angle neutron scattering to characterize the local crystallinity of the motif structures. The motif structures were found to displace much of the pure amorphous polymer with a crystalline interphase, resulting in a composite with extremely high stiffness and strain-to-failure, while also increasing the usable temperature range by 100°C. These results have important Army implications, particularly for situations where advanced materials are needed to perform in extreme thermomechanical environments.

Further, recent collaborations established with ARL helped map the local behavior around the crystalline interphase regions, revealing for the first time the nano-/micro-scale mechanical behavior of the composite motifs. The ARL group used an atomic force microscope to probe the mechanical behavior of the composite with nanoscale resolution. Further testing at ARL explored the motif behavior around a similar material system that incorporated carbon nanoparticle "bucky-balls" (Figure 1). These results provided key insight into the material property gains seen on the macroscale and provide new tools for advanced composite processing.

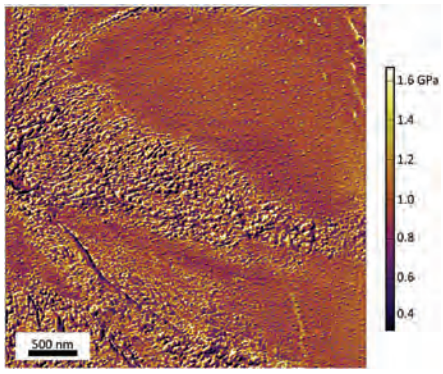

Figure 1: Mechanical behavior of a motif pattern in a polyetherimide carbon nanoparticle composite, as determined through atomic force microscopy.

Way Ahead

This ARO investigation enabled a new approach to advanced composite design: Use the fundamental understanding of the composite interphase to improve mechanical performance not through matrix-filler load transfer, but through motif structures that confine the polymer chains to more mechanically-favorable orientations. Initial efforts were focused on 2D filler systems (SWCNTs), but the team is also exploring 1D filler systems such as carbon 'bucky-balls' with the help of ARL researchers. In addition, an integrated hot stage for a transmission electron microscope at the PI institution will allow for the observation of the motif structure development over time, further guiding advanced polymer crystalline growth models.

SUCCESS STORY

Elastic Wave Cloaking

This ARO initiative resulted in a **foundational theory for creating mechanical "cloaks", or regions invisible to elastic waves,** which could provide a transformative means for protective materials, including Soldier protection, vehicle armor, protection of sensitive electronics, and other resilient structural materials

Challenge

Making objects "invisible" to various types of electromagnetic waves has been a subject of intense research for the last two decades. Groups have also explored "cloaking" for a variety of other scientific fields, including optics, thermodynamics, and acoustics. More recently, researchers have explored the possibility of mechanical wave cloaks, which could essentially make regions of an object "invisible" to elastic waves.

Many Army material systems are exposed to intense mechanical waves. Armor for Soldier or vehicle protection must withstand severe stress waves over very short timeframes; vehicle structures and electronics are exposed to intense mechanical vibrations over a wide frequency spectrum. Strategies for mitigating mechanical waves often include making structures larger or heavier, which may reduce Soldier and vehicle mobility.

To protect human and materiel assets from future threats, while also enabling extraordinary maneuverability, new strategies are required for controlling mechanical stress waves. If successful, elastic cloaking materials could provide a transformative strategy for military planners to protect Soldiers, vehicle structural components, and sensitive electronics from intense mechanical stress waves.

Action

This effort originated during a site visit to Georgia Institute of Technology in 2015. After delivering an invited talk, the Mechanical Behavior of Materials program manager Dr. David Stepp met with several faculty members individually to discuss their research ideas. During this time, he met Professor Arash Yavari, a professor in the Civil and Environmental Engineering Department, who proposed an innovative idea related to elastic wave cloaking, or ways to steer stress waves around a particular area in a body, essentially producing an "invisibility cloak" for mechanical waves. The dialogue went on for several months, with Dr. Stepp and Professor Yavari iterating until the approach and impact of the high risk idea were clear. Dr. Stepp then invited a proposal for a Short Term Innovative Research (STIR) effort. The proposal received very high reviews from both academic and Army evaluators. The STIR effort made significant progress in developing the analytic, or mathematically exact, solution to the elastic wave cloaking problem. In 2018, Dr. Stepp encouraged Professor Yavari to submit a full proposal on the topic and further develop the mathematical conditions necessary for steering stress waves in several elastic body situations, including a cylindrical hole and a spherical cavity in a body, multiple holes within a body, and a region near the surface of a body. As a first step to spur Army interest in these potentially transformative efforts, Dr. Stepp and an ARL technical advisor to the MBM program, Dr. Dan Cole, organized a joint seminar for Professor Yavari at ARL APG in

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Protection Sciences

Materials and Manufacturing Sciences

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early 2019. Professor Yavari met with several Army scientists following the seminar and discussed ways to experimentally demonstrate a simple elastic wave cloak.

Recognizing the potential Army impact of steering elastic waves, Dr. Stepp pursued a parallel path for this work with researchers at the University of Missouri, led by Professor Guilong Huang. Professor Huang proposed an idea for using metamaterials to give scientists new tools for controlling mechanical stress waves. Professor Huang's team proposed using a graded metamaterial lattice approach, which Dr. Stepp determined to be a potentially practical means for realizing an elastic wave cloak. The proposed metamaterial approach was funded as a separate single investigator award in 2018 in order to attack the elastic cloaking problem from multiple directions.

Result

These scientific investigations explored the potential for creating materials with the ability to steer mechanical stress waves around a protected region within an object. Imagine taking an object – the backing of an armor plate or the wing of an unmanned aerial vehicle (UAV) - and modelling this body as set of small cubes, often referred to as 'elements'. As forces act on the surface or body elements (e.g. projectile impacting the face of the armor plate, or airflow forces acting on the UAV wing surface), the loads are transmitted through the object onto neighboring elements. Depending on the properties of these elements (e.g. stiffness, Poisson's ratio, yield strength), engineers are able to determine the resulting mechanical behavior at various points within the body, for example the strain fields throughout the object, or the formation and growth of fractures. In the limit in which these elements become infinitesimally small, the object can be considered completely continuous and the mechanical behavior at individual points within the object can be determined.

The original elastic wave cloaking effort funded by the MBM program sought to determine the possibility of steering mechanical waves around a protected region within a continuous solid. Professor Yavari's work examined several cloaking scenarios, including shielding an internal cavity or multiple internal cavities from forces that remain constant as well as forces that vary over time. The initial result of this research determined that steering elastic waves around protected regions in continuous bodies is generally not possible if the waves vary over time, although certain special cases did appear possible. For example, in two dimensions, cloaking a hole within the body is possible if the loads are transmitted only in plane, which may have important applications for protecting regions within a thin plate. In addition, three dimensional elastic cloaks that shield cylindrical and spherical cavities may be possible within structures exposed to static mechanical loads.

Notably, these initial models do not account for mechanical metamaterials, which have mechanical behavior highly dependent on structure rather than just material properties. For example, certain structures when subject to compressive loads will actually respond by contracting instead of "popping out" (i.e. materials that exhibit negative Poisson's ratio). In addition, while exact mathematical solutions may appear to prevent the generalized elastic cloaks, approximate solutions could be possible by creating gradients in elastic properties (e.g. material stiffness and Poisson's ratio) throughout the body. Professor Huang's work used a metamaterial approach to test this hypothesis. The elastic cloak consisted of a radial gradient of lattice-based metamaterials. The

Results

- Mechanical stress wave steering theory developed for static and dynamic force application
- PI gave invited seminar at ARL in 2019
- Metamaterial approach to stress wave steering established through simulation

geometry of the lattice was such that the elastic properties did not vary if the body was rotated, but the elastic properties did vary as a function of distance from the center of the body (Figure 2A). The central void of the body was the cloaked area ($r < r_i$), while the cloak itself was contained within the graded region consisting of the metamaterial lattice structure ($r_i < r < r_c$) (Figure 2B). The researchers assumed the mechanical forces originated in the region $r > r_c$.

Through simulation, the researchers subjected the body to a simple plane wave and observed the resulting displacement fields to determine the merit of the elastic cloak. The model showed that, for a finite number of graded lattice layers, the cloaking area disrupts the elastic waves; as the number of lattice layers increases, the elastic waves were further scattered around the cloaked areas. In the limit that the number of lattice layers approaches infinity, the performance of the cloak almost entirely shielded the protected core.

To be clear, these high risk research efforts have explored the possibility of steering elastic stress waves around a particular volume or volumes within a body. Plasticity, or the point at which the yield stress is reached and the material is permanently damaged, is not considered. However, the science being developed in these projects could give military planners powerful new tools to protect human assets as well as sensitive equipment.

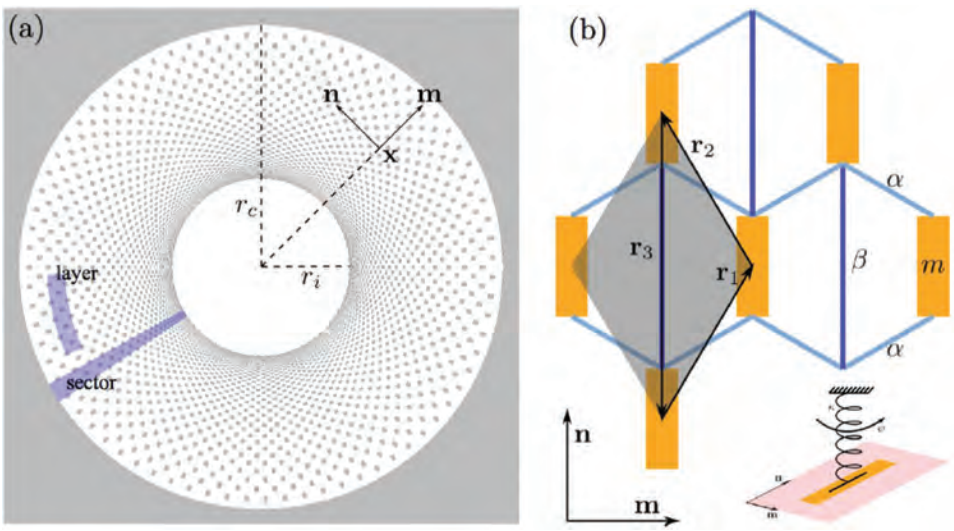


Figure 2: (a) Schematic of a body containing an elastic cloak within a central cavity; material within the radius $r < r_i$ is "invisible" to mechanical stress waves applied outside of the radius $r > r_c$. (b) Schematic of the elastic cloak layer ($r_i < r < r_c$) consisting of metamaterial lattice structure.

Way Ahead

Both of these mechanical wave steering efforts have been focused on developing the theory behind elastic cloaks, performing simulations, and guiding researchers to particular scenarios in which cloaks may be possible. Future work will attempt to experimentally demonstrate an elastic cloak using these simulations as a guide, and in collaboration with CCDC ARL. These efforts will continue in FY20 under the direction of the new Mechanical Behavior of Materials program manager, Dr. Dan Cole.

Physical Properties of Materials Program

Current Scientific Objectives

01

Create materials of novel compositions and structures with unique physical properties through developing fundamental understanding of nucleation/growth mechanisms that if successful is anticipated to lead to low power electronics and unique sensors

02

Invent unique characterization techniques and discover novel functional properties (electronic, photonic, magnetic and thermal) of materials through establishing composition/structure-property correlations that could enable new paradigms for communication, sensing, and lightweight power

Program Manager

Dr. Chakrapani Varanasi
Program Manager, Physical Properties of Materials
Division Chief, Materials Science
ARO Engineering Sciences Directorate

Dr. Varanasi completed his M.S. in Materials Science and Engineering at the Indian Institute of Technology, Kanpur, India in 1990. He trained as a Materials Scientist at the University of Notre Dame, receiving his Ph.D. in Materials Science & Engineering in 1994. He came to ARO in 2009 as the Program Manager for the Physical Properties of Program and was promoted to Division Chief, Materials Science Division in 2017.

SUCCESS STORY

Polar Skyrmions in Advanced Materials

ARO initiatives resulted in the **discovery of polar skyrmions in oxide superlattices**, creating a possibility to develop future highly efficient data storage and information processing systems.

Challenge

The impending demise of Moore's Law, the techno-economic framework that drove innovation for more than sixty years in the microelectronics industry, is leading to the search for the next generation of information processing and storage systems. Among a large number of possible fundamental pathways, magnetic skyrmions (unique textures of magnetic dipoles) are currently being investigated for low power, high-density future data storage applications. However, electric field control of such skyrmions at room temperature

This success supports these ARL Core Technical Competencies:

Network and Information Sciences

Materials and Manufacturing Sciences

Computational Sciences

and their size reduction is a tremendous challenge. The electrical analogues of magnetic skyrmions offer the possibility of small size at room temperature as well as easy control with an electric field. Nevertheless, the appropriate material systems and conditions to enable the robust study and development of skyrmions have long remained allusive.

Action

The Program Manager of the physical properties of materials program, Dr. Pani Varanasi, initially supported a theoretical proposal in 2013 from Professor Bellaiche of the University of Arkansas. The objective of this proposal was to discover several novel static and dynamical phenomena of fundamental and technological importance in ferroelectric and multiferroic ultra-thin film materials. This work resulted in the prediction of polar skyrmions in ferroelectric systems in 2015. Professor Bellaiche's calculations showed that it is possible to produce skyrmions in materials in certain conditions (proper choice of the compositions and structures). Based on these theoretical results, Dr. Varanasi identified and supported a high-risk high-payoff experimental effort to fabricate and demonstrate these skyrmions. Professors Ramamoorthy Ramesh of UC Berkeley and Darrell Schlom of Cornell University teamed up to synthesize ferroelectric oxide superlattices in hopes of realizing polar skyrmions. Although these researchers are world experts in oxide materials growth, the formation of polar skyrmions turned out to be a far more difficult task than anticipated.

Dr. Varanasi met with the PIs regularly to discuss the challenges and monitor the progress carefully. He decided to continue the support for three years of the grant, despite many setbacks and unexpected challenges, as he assessed that this team was on a right track and significant progress toward the goal was being made. Dr. Varanasi's own experience with oxide materials growth also helped him to understand the challenges well and provide expert assessment of the approach that the team was taking. This strategy of careful, regular assessment of the progress, feasibility and risk/reward of the effort allowed Dr. Varanasi to be proactively patient for the science to progress.

Result

In 2019, the experimental team has shown for the first time that it is possible to create polar skyrmions in oxide superlattices confirming the theoretical predictions. This discovery was published in the journal *Nature* (a premier journal across all scientific disciplines) and several press releases (including CCDC ARL) were made about this work. This team was able to successfully control the strain at the interfaces of materials of appropriate composition which was a crucial step to observe polar skyrmions for the first time. Using a combination of several state-of-the-art experimental techniques, including atomic-resolution electron microscopy, resonant X-ray spectromicroscopy and X-ray scattering techniques, coupled with computations, the team demonstrated the fundamental origins of the structure of each skyrmion (Figure 1).

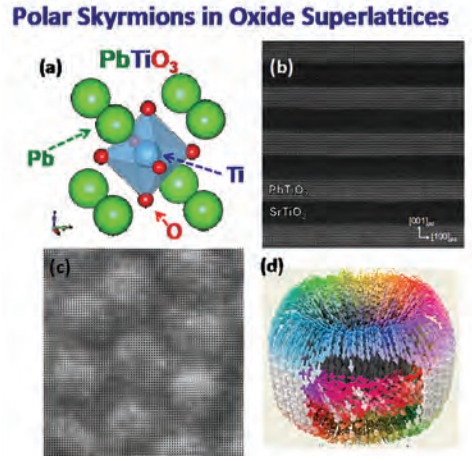


Figure 1: (a) a schematic $PbTiO_3$ perovskite crystal structure (b) An atomic resolution image of a superlattice synthesized out of the ferroelectric $PbTiO_3$ and the non-ferroelectric sister compound, $SrTiO_3$, illustrating the power of modern epitaxial synthesis techniques such as MBE and laser MBE to control synthesis at the atomic scale; (c) is a planar section electron micrograph of the skyrmions (the circular features are the skyrmions), with a lateral dimension of ~8nm; (d) is an ab initio calculation of the 3D dipolar structure of the skyrmion, with the in-plane Bloch component (shown by the RED arrows going from left to right), that shows that the skyrmion is "handed" or Chiral.

Results

- ARO co-initiated a new basic research field likely to impact future Army applications in information storage
- Achieved first theoretical and experimental demonstration of novel electrical dipole textures (polar skyrmions) in oxide superlattices
- Papers published in high impact journals and press-releases with significant attention from the research community

Way Ahead

Although the possibility of forming polar skyrmions is demonstrated, there are still many other questions that remain to be answered. The dynamics of polar skyrmions, how they interact with defects and/or with other complex dipolar structures, a comprehensive understanding of electrical topological defects and possible devices are yet to be determined. Such skyrmions present an unprecedented opportunity to translate fundamental materials physics based discoveries into technologies that could impact the DoD infrastructure through multiple pathways (including electrical adaptation and ultralow power electronics). CCDC ARL S&Es (SEDD) are aware of the recent results. New collaborations between extramural researchers and CCDC ARL S&Es will be actively facilitated to accelerate the technology transition to the Army.

SUCCESS STORY

Materials with Extraordinary Spin/Heat Coupling

An ARO initiative in spin caloritronics theory and characterization techniques has **broadened the class of materials in which thermally-driven spin transport**, and spin driven thermal transport can be developed for future applications.

This success supports these ARL Core Technical Competencies:

Network and Information Sciences

Materials and Manufacturing Sciences

Computational Sciences

Challenge

The discovery of a fundamentally new energy conversion process is a rare event. In the early 2000s, experimentalists demonstrated a new thermodynamic effect where the flow of heat in a magnetic material generates a flow of electron spin, essentially a flow of magnetic moments. These observations took the name “spin-Seebeck effect” in analogy with the well-known coupling between heat and electricity that underlies the operation of thermocouples and thermoelectric generators. The spin-Seebeck effect promised new avenues for manipulating magnetism, and a new approach for generating electrical power from a temperature difference. Theoretical understanding of the spin-Seebeck effect and related phenomena, collectively referred to as “spin caloritronics”, developed slowly. The community of scientists studying spin caloritronics effects consisted predominately of physicists from the field of magnetic devices who were less well-versed in measurement and understanding of heat transport. Influence of material compositions, structures, interfaces between materials and defects on spin-caloritronic properties were not well understood and had only been demonstrated in a few very specific material systems.

Action

To understand the basic mechanisms to create materials with extraordinary spin/heat coupling, the Program Manager of Physical Properties of Materials, Dr. Pani Varanasi, identified and supported a new research effort proposed by Professor David Cahill of the University of Illinois Urbana-Champaign to study thermal conductivity due to magnons in certain oxide materials. Based on the success of this project, Dr. Varanasi also

successfully advocated for a new MURI project in collaboration with Dr. Mark Spector of ONR to study systematically the phenomena of Spin Caloritronics (phonon-magnon coupling, magnon-defect interactions, etc.) in a wide range of materials. A MURI team formed in 2012 led by Professor Roberto Myers at Ohio State University brought together experts in the physics of spin and heat transport in materials. The main objective of this project was to develop a fundamental understanding of spin-heat coupling in solids through coordinated research in theory, experiment, measurement science, and new materials. Dr. Varanasi recognized the importance of bringing together researchers from different research groups, both in U.S. and abroad, to accelerate the progress of an emerging area. He supported several workshops organized at different locations (2015, 2017, and 2018) that bought together leading domestic as well as international researchers to exchange ideas and discuss results in the new field of Spin-Caloritronics. In addition, Dr. Varanasi supported several single investigator awards and also specialized instrumentation through the DURIP program to augment research in this area and to explore several other several materials systems that were not covered by the MURI team.

Result

The ARO supported researchers experimentally discovered and theoretically predicted several breakthrough spin-heat conversion effects. Before the ARO initiative, the conversion of heat to electrical power by the spin-Seebeck effect was known to be a three-stage process: i) generation of spin currents by temperature gradients; ii) transport of spin across an interface between a ferromagnetic insulator and a normal metal; and iii) conversion between spin and charge currents by the relativistic effects of spin-orbit coupling. The ultimate goal was to understand the properties of materials that govern each stage of this energy conversion process. The researchers also targeted materials where large useful energy conversion might be realized, such as giant spin-Seebeck signals on order ~10 mV K^{-1} (100 times larger than typical Seebeck effects in thermoelectric materials) and giant magnon thermal conductivities as large as the thermal conductivity of metal alloys.

The MURI team was able to develop the basic physics of spin/heat interactions in materials. Building on these foundations, new experiments, materials, and theory have been developed, including, all-optical thermometry using nitrogen-vacancy centers in diamond (Figure 2) , ultrafast demagnetization across metallic interfaces (Figure 3), vortex-mediated transport between magnets and superconductors, and spin/heat coupling in disordered and low dimensional systems.

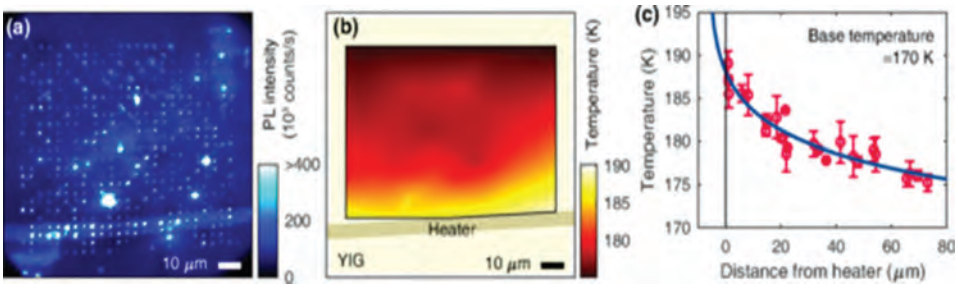


Figure 2: Temperature mapping using NV-centers in diamond on YIG, published in Physical Review Applied, July 2019

Results

- More than 120 publications in high impact/reputed journals in a new field of Spin-caloritronic Materials
- Young researchers (students, postdocs) trained in this novel area with the ARO support are now conducting research in various key positions globally
- A new phenomena of pho-spin voltaic effect was discovered (Professor Wu, Colorado State University)
- ARO funded discoveries directly led to new or expanded investments at NSF and DoE research centers

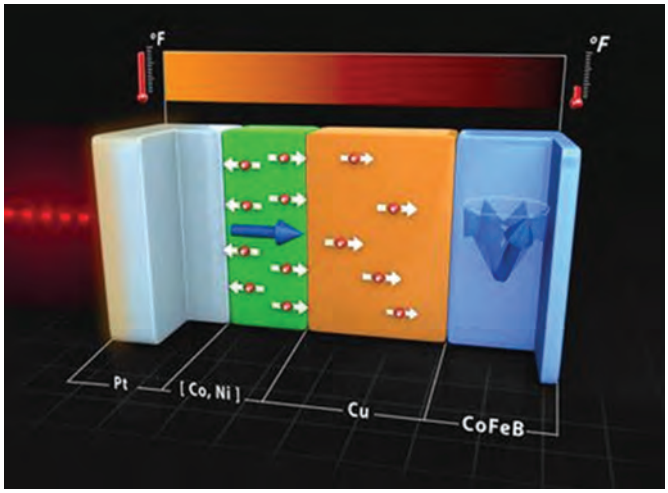


Figure 3: Schematic of the ultrafast thermal spin-transfer torque effect, published in *Nature Physics*, June 2015

The ARO funded expansion of spin caloritronics theory and characterization techniques has strongly broadened the class of materials in which thermally-driven spin transport, and spin driven thermal transport can be developed for future applications in thermal management, waste-heat recovery, and spintronics. The thermally-pumped Bose-Einstein Condensate (BEC) agenda propelled by the MURI has impacted the developments in the broader spintronics/spin-caloritronics community, leading to novel magnon BEC realizations by other groups utilizing thermal/spin conversion processes.

These results led to the launch and investments at a range of U.S. research centers, including:

Renewal of the NSF Materials Research Science and Engineering Center (MRSEC) at Ohio State University in 2014 (led by Heremans; MURI co-PI) largely inspired by work funded under the MURI

Established the NSF MRSEC at Univ. of Illinois in 2017 (led by Cahill; MURI co-PI), about metallic antiferromagnetic materials. MURI support was instrumental in advancing studies that led to the creation of this center.

Established the DoE Energy Frontier Research Center called Spins and Heat in Nanoscale Electronic Systems (led by Professor Jing Shi at UC Riverside) with research focused on spin/heat transport in nanoscale materials

Way Ahead

Although significant progress in basic understanding of spin caloritronics has been accomplished, there are still technical challenges remaining to realize practical applications. Strategic investments in extramural basic research will be made to address these challenges and achieve high figure of merit of energy conversion exploiting spin-caloritronics in different materials. Collaborations with the CCDC ARL S&Es will be actively pursued for accelerating the technology transfer to the Army.

Synthesis and Processing Program

Current Scientific Objectives

01

Understand how processing methods and conditions influence the features and properties of structural materials, and how these influences can be leveraged for superior mechanical performance. If successful, this will enable sophisticated synthesis of advanced structural materials to protect the Soldier and Army materiel that are stronger, lighter, and higher performance than the current state of the art.

02

Develop new materials processing methods utilizing far-from-equilibrium and metastable conditions to create new phases and enable new synthesis strategies for creating advanced materials concepts; successful development of advanced processing methods will make possible material concepts that are currently unrealizable, enabling synthesis of materials with unprecedented capabilities for the future Soldier.

03

Investigate the fundamental physical laws that occur during materials processing, with the goal of characterizing and defining previously ill-understood phenomena and behavior that if successful will enable advanced and efficient materials fabrication processes to create more sophisticated materials and eliminate undesirable influences that cause flawed or sub-standard materials in Army materiel.

Program Manager

Dr. Michael Bakas

Program Manager, Synthesis and Processing
Materials Science Division
ARO Engineering Sciences Directorate

Dr. Michael Bakas obtained his Ph.D. in 2006 in Ceramic & Materials Science Engineering from Rutgers University. He arrived at ARO in 2015 as a SETA Contractor, and in 2017 was appointed Program Manager of the Synthesis and Processing Program.

SUCCESS STORY

Technical Foundation Established for Synthesis of Advanced Coatings and Energetics via Dusty Plasmas

ARO PMs **identified to leverage existing plasma physics knowledge** to develop new processing method for materials and

This success supports these ARL Core Technical Competencies:

Ballistics Sciences

Materials and Manufacturing Sciences

This success was made possible by the following ARO S&Es or Program Specialists:

- Dr. Michael Bakas, ARO Materials Science Division
- Dr. David Stepp, ARO Engineering Sciences Directorate
- Dr. James Parker, ARO Chemical Sciences Division

energetics that will **enable creation of more energetic explosives and propellants.**

Challenge

As researchers attempt to create the next generation of structural materials, it is becoming increasingly clear that pushing the performance envelope is going to require introducing unique engineered microstructures and phases that necessitates synthesis methods with dramatically enhanced positioning and precision. Historically, bulk structural materials processing is primarily based on application of thermal energy and pressure, and these tools have been limited to a coarse level of control. This issue is also present in energetic materials, where high energy nanoparticles need to be synthesized and coated in an inert controlled environment in order to preserve their potential energy. New methods and approaches that enable a greater level of precision are needed for fabricating bulk structural materials and high performance energetic materials.

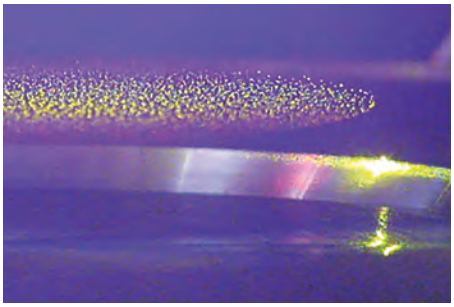


Figure 1: Polymer particles arranged in a plasma crystal.

Action

In 2016, Dr. Bakas became aware of a field of study in plasma physics focused on the creation of "plasma crystals." Plasma is the fourth state of matter, in which electrons and nuclei are completely unbound, creating a sea of negatively charged electrons and positively charged ions. Some plasmas, called "dusty" plasmas, retain solid matter particles within them. Plasma physicists learned that these particles develop a charge due to interacting with the plasma environment, and these charges could be manipulated to arrange said particles in an ordered lattice, similar to an atomic crystal structure. These arrangements were called "plasma crystals" (Figure 1), and multiple physicists have published results in this area.

Dr. Bakas and Dr. Stepp consulted with Dr. James Parker, of the Molecular Structure and Dynamics Program, and Dr. Richard Hammond, then program manager for the Optical Physics and Fields program, to develop a MURI topic to explore the use of dusty plasmas and plasma crystals for materials processing. The team had discussions with astrophysicists, fusion energy researchers, and materials researchers, and eventually came to the conclusion that not only was the idea plausible, it also was not currently being explored in the research community. The ARO PMs drafted a MURI topic in 2017 that was selected by the Office of the Secretary of Defense for the Fiscal Year 2018 MURI BAA.

Result

The winning MURI proposal was from a team led by Professor Uwe Kortshagen of the University of Minnesota, and consists of University of Michigan Professors Mark Kushner and Angela Violi, University of Iowa Professor John Goree, Caltech Professor Harry Atwater, and University of Washington in Saint Louis Professor Elijah Thimsen. The team presented an overall strategy of creating particles in the plasma, driving particle agglomeration by modulating the plasma to create positively and negatively charged particles, and then consolidating these particles agglomerates in an organized manner using plasma crystal inspired manipulation. Thus far, the MURI team has demonstrated that particles in a plasma

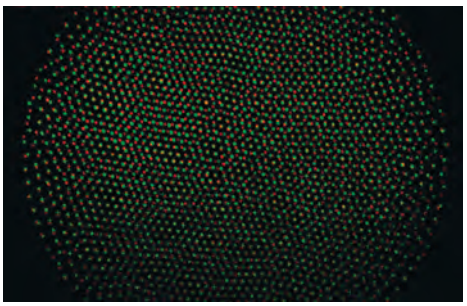


Figure 2: Position of particles initially (red), and prior to impact (green), in dusty plasma experiment.

crystal maintain their formation during the free fall that occurs after an electric field is removed (Figure 2), and coatings with directional scattering and unique radiative cooling can be created by exploiting the capabilities of dusty plasmas to vary composition and fill volume in films.

The MURI effort was initially funded in 2018. In attendance at the kickoff meeting was Dr. Chi-Chin Wu, a research scientist of CCDC ARL WMRD. Dr. Wu recognized the potential of dusty plasmas to create unique energetic particles. In addition, she recognized that a dusty plasma consolidation processing method may enable advanced energetic materials synthesis by enabling synthesis and coating of nanoparticles in a controlled environment. Dr. Wu worked with ARL Central to support a post doc at University of Minnesota, Dr. Katharine Hunter, to explore the synthesis of coated aluminum particles using dusty plasmas that could potentially be utilized for advanced energetic materials.

Way Ahead

The preliminary results are very promising for establishing a novel dusty plasma processing technique, especially the demonstration of high thermal radiation coatings, which will be published in the scientific literature. Furthermore, the collaborations within CCDC ARL will seek to fabricate unique high energy nanoparticles to enable advanced explosives and propellants for the Army.

Results

- ARO is driving multidisciplinary studies with transition paths in place within CCDC
- Demonstrated ability to retain particle position upon field removal and synthesis on unique photonic and thermal coatings
- Academic expertise initially funded through ARO transitioned to ARL Central to provide ARL with expertise in dusty plasmas, for the synthesis of high energy nanoparticles for energetic materials

SUCCESS STORY

Means of Inducing Ductility into High Strength Brittle Materials Discovered

Single Investigator grants supported by the Synthesis and Processing program uncover mechanisms for **mitigating brittleness in high strength nanomaterials,** laying the foundation for future Army structural and protective systems.

Challenge

Creating higher strength materials is always of interest to the Army, as such materials enable superior structural and protective systems. One common means of improving strength has been to reduce the grain size. Hall-Petch theory states that the strength of a material will increase as the grain size decreases, but the tradeoff is a reduction in ductility. This is caused by many factors, but a significant reason is that metals deform plastically by dislocation motion and the more numerous grain boundaries that come with a smaller grain size impairs this motion. As the grain size of materials approaches the nanoscale, new means on inducing ductility must be found to assure they possess the requisite durability and toughness. Otherwise the brittle failure that occurs will prevent the future use of nanograined materials, despite their high strength.

This success supports these ARL Core Technical Competencies:

Protection Sciences

Materials and Manufacturing Sciences

This success was made possible by the following ARO S&Es or Program Specialists:

- Dr. Michael Bakas, ARO Materials Science Division
- Dr. David Stepp, ARO Engineering Sciences Directorate

Results

- Identified two means of inducing ductility in nanocrystalline alloys: amorphous grain boundaries and amorphization induced shear bands
- Discovered possible source of inverse Hall-Petch behavior observed in yttria-stabilized zirconia
- Fabricated of nanocrystalline bodies greater than the microscale that retain ductile behavior

Action

Dr. Bakas initiated extramural grants in the ARO Synthesis and Processing program focused on exploring the causes of brittleness in fine-grained materials, and processing solutions to mitigate them. One of these grants was awarded to Professor Szlufarska at the University of Wisconsin who had proposed a combined experimental and computational study into the wear of nanocrystalline alloys. Dr. Szlufarksa planned to perform nanomechanical experiments in an atomic force microscope and utilize molecular dynamics simulations to interpret and understand the experimental results. Another effort was started with Professor Timothy Rupert at the University of California, Irvine. Professor Rupert had a program in 2012, managed by the former Synthesis and Processing program manager Dr. David Stepp, to explore fabrication of nanocrystalline alloys. In that work, he demonstrated that amorphous grain boundaries in nanocrystalline alloys increased ductility in micropillars by enabling dislocation absorption. In 2016, Dr. Bakas awarded a new grant to try to create larger nanocrystalline bodies with the amorphous grain boundaries, as the samples in the previous work were fabricated using an unscalable process. Dr. Bakas initiated another grant in 2018 with Professor Ricardo Castro and the University of California, Davis. This work was focused on discovering the causes of inverse Hall-Petch behavior, the point at which smaller grain size no longer improves strength, in ceramic materials.

Result

In 2019, Professor Rupert demonstrated the fabrication of >99% dense Cu-Zr samples with ½ inch diameter using conventional hot pressing methods. The nanocrystalline grain structure with amorphous boundaries was retained, and micromechanical testing demonstrated they retained the same level of mechanical performance as the smaller ball milled samples. Professor Rupert has filed a patent on this process. Professor Castro was able to observe grain boundary sliding in yttrium-stabilized zirconia using in-situ electron diffraction in an SEM. This suggested the nanocrystalline ceramics were undergoing a form of creep, which normally is observed only at high temperatures. While this resulted in a lowering of the material's hardness, it may be a means to induce more plasticity in the ceramic.

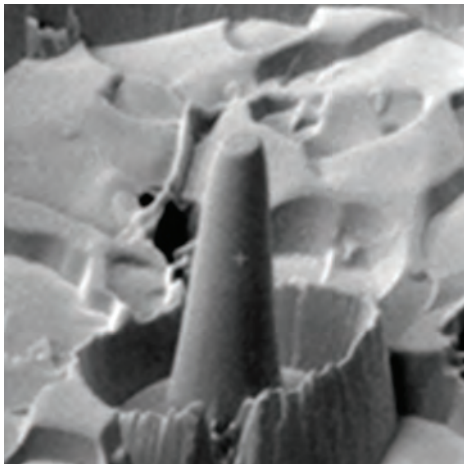


Figure 3: Micropillar experiment showing ductile deformation in $SmCo_5$ despite the lack of dislocations.

Additionally, a stand out result was attained in 2019 by Professor Szlufarska. In 2018, the molecular dynamics simulations on the $SmCo_5$ she was working on predicted the material would behave in a ductile fashion, but the stresses applied in the simulation would not form dislocations or move them. The simulations predicted that at the smaller grain sizes inherent to a nanocrystalline alloy, stresses would build up within the grain, creating a shear band that would cause the material to lose its ordered structure, a phenomena called amorphization. These amorphous shear bands served as an accommodation

mechanism, causing the boundaries to slide and the material to plastically deform. This amorphization driven plasticity was confirmed experimentally with micropillar experiments (Figure 3). This is a potential alternative to dislocation driven plasticity and would not be impaired by small grain sizes. A publication on the topic was accepted and published in *Nature Communications* in 2019.

Way Ahead

The amorphization mechanism has so far only been confirmed in one material, $SmCo_5$, which is not a structural material. The conditions that cause the amorphization driven plasticity need to be better defined and created in alternative material systems. Potential linkages to the low temperature creep observed by Professor Castro in ceramics will be explored. The program managers of Mechanical Behavior of Materials, Synthesis and Processing, and Solid Mechanics will coordinate their efforts to support multidisciplinary collaborations to further extend this work, in collaboration CCDC ARL.

Complex Dynamics and Systems Program

Current Scientific Objectives

01

Discover general principles governing the dynamics and control of moderately high-dimensional and strongly coupled interacting systems. If successful, this research could lead to a massive change in DoD tools to perform design, pursue inference from data, and control for a class of systems possessing a very broad set of nonlinear features

02

Control the underlying geometry, information flow, and energy in nonequilibrium dynamical systems that if successful, will lay the foundations for developing nano-scale systems capable of coordinating molecular assembly of materials and systems with novel properties, and a generation of denser, faster, cheaper, and more energy efficient computing devices

03

Discover and shape hierarchical interactions leading to emergent phenomena in programmable active matter and complex collectives that if successful, this will enable new understanding of the mechanics of naturally occurring active soft matter that could be translated to synthetic systems and materials with active microstructures of Army and DoD relevance, such as modular and soft robotics, reconfigurable assemblages of autonomous swarms, and adaptive, reconfigurable materials

04

Control intrinsic activity and potential energy landscapes to engineer novel adaptive nonlinear meta-structures that if successful, may lead to complex material and structures for actuation, vibration protection, and shock mitigation in ground and air vehicle technologies

Engineering
Sciences
Directoriate

- Electronics Division
- Material Sciences Division
- **Mechanical Sciences Division**

Program Manager

Dr. Samuel Stanton
Program Manager, Complex Dynamics and Systems
Mechanical Sciences Division
ARO Engineering Sciences Directorate

Dr. Stanton completed his undergraduate studies at the U.S. Naval Academy, receiving his B.S. in Aerospace and Astronautical Engineering in 2004. He completed his graduate training at Duke University, receiving his M.S. and Ph.D. degrees in Mechanical Engineering in 2008 and 2011, respectively. He came to ARL in 2011 as the manager for the Complex Dynamics and Systems Program and additionally served as Acting Program Manager for Multi-Agent Network Control for several years.

SUCCESS STORY

The Inception of the "Information Engine"

This ARO initiative resulted in **fundamental understanding of how information can be leveraged as a resource to do physical work** as well as how energetics and fluctuations lead to emergent patterns.

This success supports these ARL Core Technical Competencies:

Network and Information Sciences

Materials and Manufacturing Sciences

Computational Sciences

This success was made possible by the following ARO S&Es or Program Specialists:

- Dr. Samuel Stanton, ARO Mechanical Sciences Division

Challenge

Army systems must operate with speed, agility, and efficiency in uncertain and constantly changing environments. Research efforts are underway to address these aspects of the Army operating environment, but there does not exist an encompassing and unifying framework describing general properties and principles. That is, how do active systems shape the flow of disorganized sources of energy into focused and useful work? Modern systems (especially robotic systems) must additionally process and generate information in addition to energy. However, traditional theories of thermodynamics, information, and dynamical systems have developed mostly in isolation from one another. In the few cases where these disciplines have intersected, they have mostly been accomplished in cases where the dynamics are fairly benign and other restrictive assumptions that are not typical of Army problems. Can these domains and approaches be integrated, purposefully transduced, and intelligently controlled in complex environments?

Action

In 2012, Dr. Samuel Stanton brought attention to recent experimental advances unifying nonequilibrium thermodynamics and information theory at the nanoscale to the research community through a Multidisciplinary University Research Initiative (MURI) topic. Therein, Dr. Stanton also identified both the need and opportunity to establish a link to control theory for intelligently managing the flow of energy and information as well. ARO selected a team led by Professor James Crutchfield of the University of California

at Davis to establish theoretical foundations unifying nonequilibrium thermodynamics, information theory, control, and dynamical systems.

Dr. Stanton orchestrated a joint MURI review in 2014 between Professor Crutchfield's effort and another MURI topic on the control of complex networks by that was pursuing a novel experimental system consisting of a network of nanoscale oscillators. Ensuing collaborative discussions revealed new opportunities to reconfigure the nanoscale oscillator platform concepts to carry out some of the first direct measurements of heat transfer to a thermal bath during a logic bit operation (on the order of zepto-Joules). In 2015, Dr. Stanton utilized the Defense University Research Initiative Program (DURIP) to enable Professor Crutchfield's MURI team to pursue collaborative opportunities with Professor Michael Roukes's experimental group at the California Institute of Technology. The team realized that to measure the energy fluctuations of such small energy within a reasonable (<1GHz) bandwidth, thermal conductance and heat capacity needed to be effectively eliminated through refrigeration. The DURIP facilitating experimental infrastructure to take temperatures to the milli-Kelvin levels essential for measurements.

Result

The MURI team was extremely successful in capitalizing on this opportunity. The team developed a broadly extensible theory accounting for the diverse kinds of information that complex nonlinear systems are capable of producing and storing as well as how certain irreversible thermodynamic processes limit computation. The experimental collaboration culminated in demonstrating that highly structured distributions of work emerge during even the simple task of erasing a single bit. The structure of the distributions were shown to track the mesoscale evolution of a system's informational states and revealed classes of microscopic trajectories that could be harnessed constructively.

The team was able to extend the theory to adaptive agents capable of processing and storing information and energy in random environments. Groundbreaking experiments have been conducted aimed at producing the first direct thermodynamic measurements of information processing in nanoscale systems. There now exist preliminary principles of thermodynamic information processing, to include a new *Information Processing*

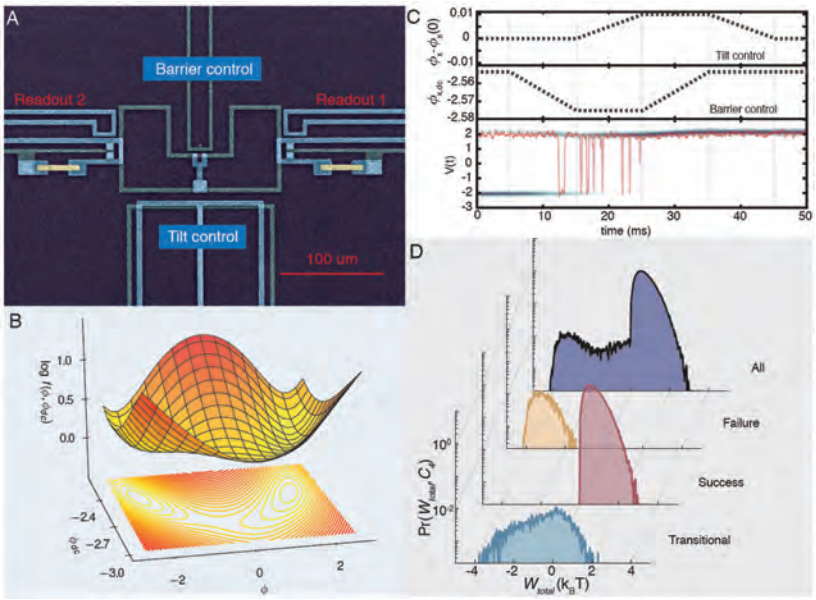


Figure 1: Implementation of metastable memory and bit erasure driven by thermal fluctuations. The interplay between magnetic inductances and nonlinear Josephson inductances gives rise to a controllable potential landscape. (A) Optical micrograph of a gradiometric flux qubit with control lines and local magnetometers for state readout. (B) Calculated potential energy landscape at the beginning of the erasure protocol. (C top) Sequence of tilt and barrier control waveforms implementing bit erasure and (C bottom) sample of resulting magnetometer traces tracking the system's internal state. (D) Structured work distributions over trajectories during a bit operation. From: https://arxiv.org/pdf/1906.11973.pdf

Results

- Published detailed analysis of how Maxwellian Demons convert disorganized thermal energy to useful work and showed that instability (deterministic chaos) drives the conversion
- Introduced a new class of information engines that use information as a thermodynamic fuel to harvest disordered energy
- Discovered an information-processing Second Law that extends Landauer's Principle of the thermodynamic costs of erasure to general computation

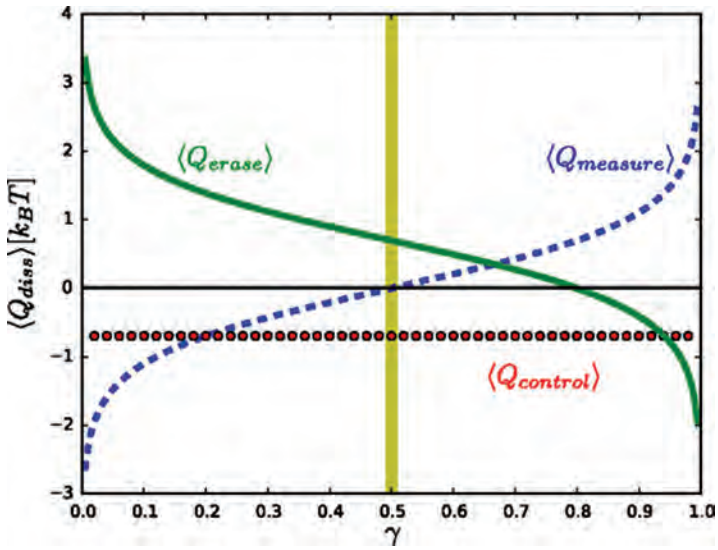


Figure 2: Trade-offs in thermodynamic costs beyond Landauer's principle: Thermodynamic costs (energy dissipation Q_{diss}) for measurement, control, and erasure in Szilard's information engine as a function of γ(demon partition). Landauer's principle is the vertical yellow band at the middle: Measurements are thermodynamically free, but erasure costs because heat is dissipated as a result of demon resetting. Costs exactly flip when γ=4/5, where erasure is thermodynamically free and measurement takes on the usual cost of erasure. From Boyd and Crutchfield, *Physical Review Letters*, Volume 116, Number 190601 (2016).

Second Law of Thermodynamics governing how physical entropy can decrease if compensated by the Shannon-Kolmogorov-Sinai entropy change of information-carrying degrees of freedom. The team derived new metrics and principles to explain the how information is stored in a dynamic system's structure, how much information can be generated, and how stored and generated information can be used to produce future desired behaviors. There is new understanding how information can serve as a reservoir akin to thermal reservoirs for doing work in nonlinear systems out-of-equilibrium.

Way Ahead

Experiments are continuing with nanoelectromechanical systems and superconducting quantum interference devices. Experiments at these length scales necessarily require consideration of intrinsic nonlinearity and fluctuations. Also, theoretical frameworks are extending traditional measures of information to statistical dependencies underlying the dynamics of complex system organization. Going forward, additional research focus areas include:

- Fundamental science of nonequilibrium thermodynamics: This is key to understanding emergent organization in a wide range of mechanical, electronic, chemical, biological, and social processes of interest to the Army.
- Fundamental science of physical information processing: Developing methods to analyze nonlinear mechanisms coupling energy and information flows in complex systems.
- Minimum energy requirements: The newly derived bounds on energy dissipation required for information processing will allow for more accurate estimates of optimal energy efficiencies in a wide range of information processing and control systems of interest to the Army.

SUCCESS STORY

Complex Emergent Behavior in Smart Active Particles (Smarticles)

ARO funding leads to demonstration of a **robot built entirely from smaller robots known as 'smarticles'**, thereby opening the door to a potentially new locomotion technique.

This success supports these ARL Core Technical Competencies:

Materials and Manufacturing Sciences

This success was made possible by the following ARO S&Es or Program Specialists:

- Dr. Samuel Stanton, ARO Mechanical Sciences Division

Challenge

The Army Functional Concept for Movement and Maneuver states that in the future, "a robotic swarm may someday be capable of moving to a river and then autonomously forming a structure to span the gap." This challenge goes far beyond traditional domains of swarming robotics where the number or robots is typically on the order of less than a dozen and the robots rarely physically interact. Extending to orders-of-magnitude larger numbers of interacting agents is challenged by our lack of ability to predict global system behaviors and performance envelopes based on interaction rules; lack of understanding of fundamental tradeoffs between system accuracy, responsiveness, and resilience; lack of a framework to build distributed control algorithms for modulating system response and optimize desired emergent properties. Furthermore, research has not considered the potential for multi-agent systems to dynamically interconnect and reconfigure in ways that are commonly seen in the nature (especially in species of ants that self-organize into rafts, towers, and bridges). Control of collectives is a significant challenge as traditional synthesis techniques rely on known input-output relationships to achieve desired behaviors.

Action

Dr. Samuel Stanton advised a 2017 DARPA seedling effort on Complex Collectives focused on elucidating the computational and noise-driven challenges. In particular, Dr. Stanton developed and co-advised DARPA on scientific problems concerning the fragility of top down algorithms, how small errors can lead to cascading error propagation, and how some emergent behaviors will only show up in physical platforms but not in idealized simulations. This program was successful in showing how top-down self-organization is possible as well as how local interaction rules for a given goal can be systematically compiled. However, the problem of physical interconnectivity and bottom-up emergence were not well addressed. Dr. Stanton began to organize the physics and control communities to work together on this problem through a workshop at Georgia Tech organized by Professor Evangelos Theodorou. Many new areas of interaction were identified, but Dr. Stanton specifically encouraged Professor Daniel Goldman of Georgia Tech's Physics Department to present his new results on optimal nest building in ant colonies and their paradoxical distributions of ant activity levels as a challenge problem for the control science community to formulate and understand. At this workshop, Professor Goldman learned of former MIT Professor Jeremy England's theory of "least rattling" in collectives as well as his postulated principles of emergent simplicity, emergent control. Dr. Stanton encouraged a collaborative seedling proposal with Professors Goldman and England to experimentally test England's theories. In addition, Dr. Stanton encouraged the use of Professor Goldman's new smart active particle robots (dubbed "smarticles") as a testbed.

Results

- Random motions of a smarticle ensemble demonstrated the first experimental evidence of emergent yet deterministic behavior
- A new form of dynamics-informed machine learning called Dynamical Systems Segmentation identified emergent control authority

Result

In 2018, Professor Goldman discovered that when geometrically confined, the random motions of his smarticle ensemble demonstrated the first experimental evidence of emergent yet deterministic behavior: the internal collisions among the smarticles and an enclosing membrane resulted in diffusive locomotion. The emergent diffusion was additionally shown to be capable of being directed in top-down manner by engineering the ensemble to respond to a light source in a manner analogous to biological phototaxis. Dr. Stanton leveraged these results to build a program of research unifying the theory of algorithms, control, and the physics of active matter to formally explore the interplay between bottom-up emergent behavior and pattern formation with top-down control.

A research breakthrough was achieved the following year. An interdisciplinary team comprised of physicists, computer scientists, and control theorists collaborated to experimentally and theoretically show that directed drift of a supersmarticle configuration could be achieved via inactivation of individual smarticles. Researchers used state-of-the-art data-driven machine learning and control tools to discover a relationship between smarticle activity and transport from a single experimental trial. This opened the door to decentralized closed-loop control of sophisticated emergent behavior in a collective of unsophisticated robots.

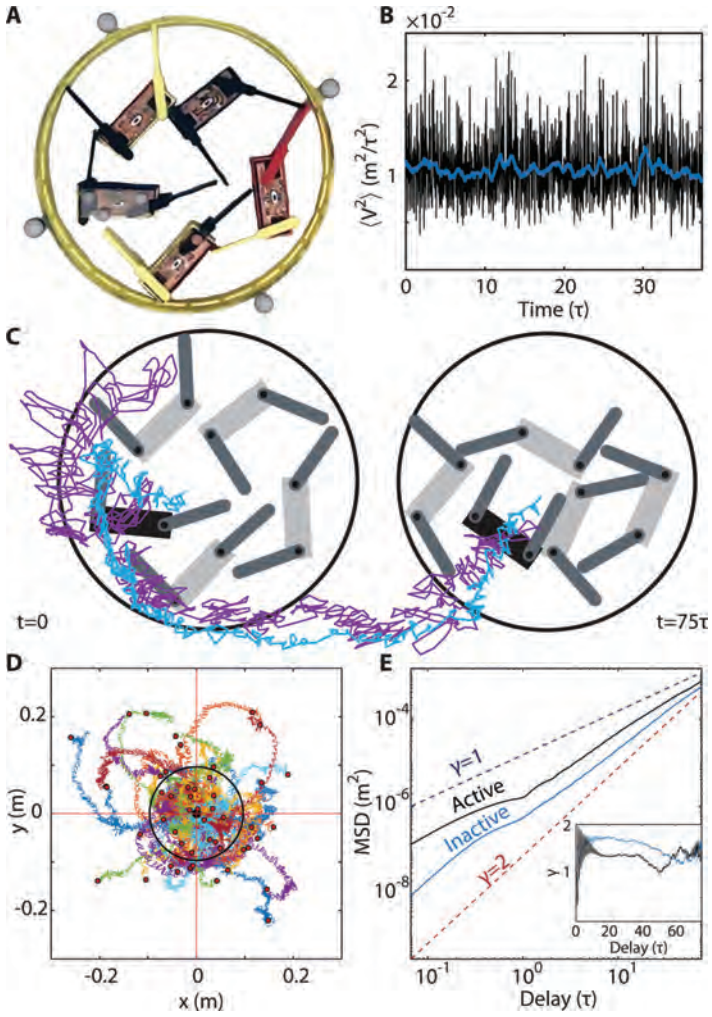


Figure 3: Collective confined diffusion with Smarticles. (A) Supersmarticle top view (B) Granular temperature of five active smarticles confined in a ring; black line is raw data over 10 trials, and blue is a moving window mean. (C) Experimental trajectories of a smarticle inside the ring (purple), and the ring's center of geometry (blue). (D) Experimental tracks of ring trajectory for 50 trials; the black circle represents the size and initial position of the ring. (E) Mean square displacement averaged over 50 and 80 trials, for the active and inactive systems, respectively. From Savoie *et al*, Science Robotics, Volume 4 (2019).

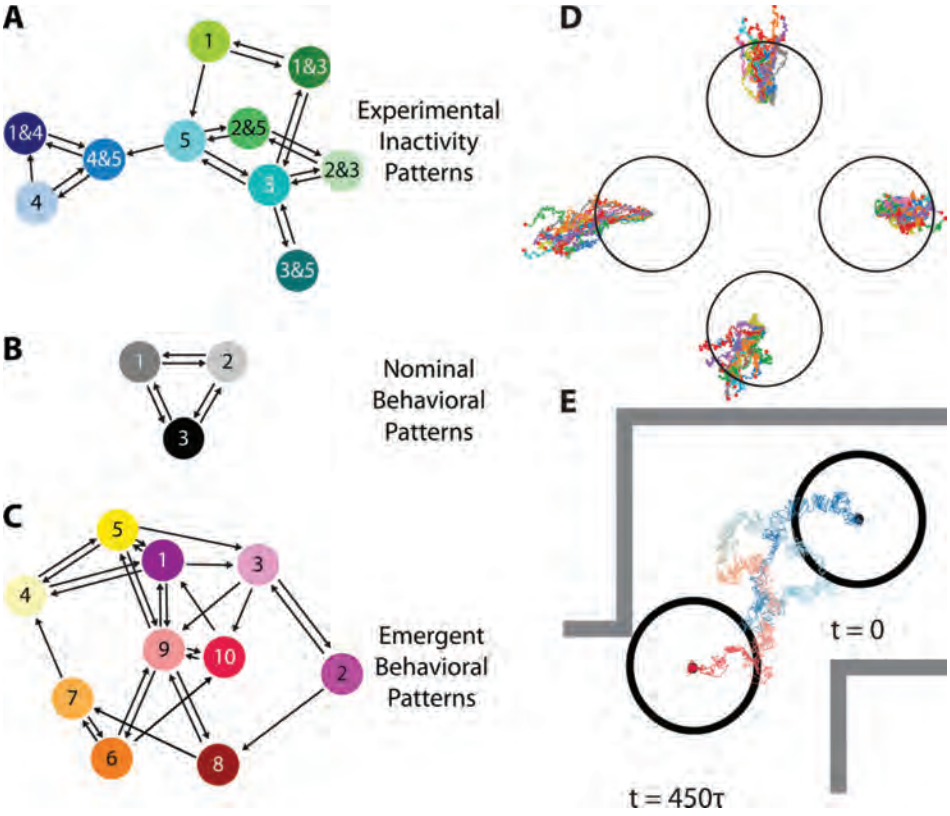


Figure 4: Comparison between observed and numerically generated behavioral patterns. (A) Model shown is a graphical representation of a single inactive smarticle switching sequence observed in a phototactic experiment. Graphical models were extracted using a Dynamical Systems Segmentation algorithm from the same experiment with and without candidate control information, shown in (C) and (B), respectively. (D) Simulated supersmarticle trajectories predict that the ensemble is capable of movement anywhere in the plane while receiving exogenous feedback from an external controller. (E) Experimental trajectory of a photophilic supersmarticle in which the system was exogenously steered through a maze by an experimenter, validating the simulation's predictions. The trajectory evolves in time from blue to red, and the black circles represent the initial and final ring configurations. From Savoie *et al,* Science Robotics, Volume 4 (2019).

Way Ahead

The "supersmarticle" research results lay the foundation for future robotic materials comprised of multi-robot systems that leverage the low-order computation and actuation to achieve system-level performance. Future work developing the algorithmic and physical foundations of emergent collective will allow for heterogenous robots to self-organize to achieve Army-relevant tasks. By considering the emergent mechanics and stresses, a path toward the visions of self-organized robot behaviors envisioned by the Army Functional Concept is at hand.

Fluid Dynamics Program

Current Scientific Objectives

01

Understand and predict the dynamics of unsteady and separated flows, identifying critical parameters or "signatures" of incipient separation events that if successful can either be used to avoid boundary layer separation or to generate large aerodynamic forces and moments to improve Army aircraft

02

Direct confrontation of nonlinear behavior inherent in the governing equations of fluid dynamics will allow global prediction capabilities (vs local), and will also permit the leveraging of nonlinearities for novel effects, thereby providing methods to improve future Army airborne systems

03

Erection of new frameworks for prediction of turbulent phenomena will overcome current stochastic methodologies that are often more descriptive than predictive, that if successful will enable new models for turbulent behavior that permit the design of leap-ahead aircraft technologies for the future Army

Program Manager

Dr. Matthew Munson

Program Manager, Fluid Dynamics
Mechanical Sciences Division
ARO Engineering Sciences Directorate

Dr. Munson completed his undergraduate studies at Illinois Institute of Technology, receiving his B.S. in aerospace engineering in 2002. He pursued doctoral studies at the California Institute of Technology, receiving his Ph.D. in aeronautics in 2012. A recipient of the DoD Science, Mathematics and Research for Transformation (SMART) Scholarship, Dr. Munson started at CCDC-ARL in 2012 as an Aerospace Engineer in the Vehicle Technology Directorate. He transferred to ARO in 2014 as Program Manager for Fluid Dynamics.

SUCCESS STORY

Understanding Galloping Instabilities of Rectangular Cylinders – Towards Drag Reduction for Precision Airdrop Systems

This ARO initiative led to **discoveries of the galloping characteristics of rectangular cylinders**, relevant to increasing performance of precision air-drop suspension-line systems.

This success supports these ARL Core Technical Competencies:

Protection Sciences

This success was made possible by the following ARO S&Es or Program Specialists:

- Dr. Matthew Munson, ARO Mechanical Sciences Division

Challenge

Parachute systems are manufactured using flexible suspension lines that are susceptible to flow-induced vibrations. These vibrations result in audible noise generation, as well as increased aerodynamic drag (perhaps up to a 60% increase over baseline). Suspension line aerodynamics is characterized by the intricate interplay between the unsteady fluid dynamics around the lines, the nonlinear mechanical response of the lines, and the presence of complex geometry. Recent studies have been unable to identify the critical parameters leading to the onset of flow-induced oscillations, especially a large amplitude oscillation known as galloping.

Galloping occurs when lateral oscillations of the line induces an unsteady variation in the angle of incidence and the velocity magnitude of the oncoming flow. The resulting unsteadiness in lift and drag leads in the transfer of energy from the flow to the line in a self-sustaining cycle. In additional to lateral oscillations, torsional galloping my also occur, resulting in unsteady twisting of the line.

Action

Dr. Munson first became aware of the impact of galloping and its effects in flow-induced vibrations during a site visit to CCDC SC. Dr. Keith Bergeron, an engineer with the precision air-drop team, wondered if there was anyone in the fluid dynamics research community who could investigate galloping in rectangular cylinders and identify both the critical parameters responsible for the onset of galloping, as well as verify the validity of assumptions made during traditional design analyses. Much of Dr. Bergeron's work had focused on the specific suspension lines currently in use, which made it difficult to identify concrete reasons for observed behaviors.

Dr. Munson identified a set of researchers at Michigan State University who had the required capacity to break the problem into a set of scientific questions and simplified experiments aimed at identifying the required parameters. In 2017, Dr. Munson recommended an award to support an effort from Professors Ahmed Naguib and Manoochehr Koochesfahani. The team is currently conducting an experimental campaign to:

- Systematically investigate the galloping stability of rectangular cylinders, specifically focused on variations in corner radii, aspect ratio and surface topology.
- Identify the limits of the assumption of quasi-steady flow traditionally used to analyze galloping. In other words, they are working to identify the significance of the dynamics.

- Combine flow-field measurements with surface pressures and force/moment data to discover the fundamental flow mechanisms that lead to the galloping behavior. Discovery of these fundamental connections could lead to simplified (but still physically grounded) models of galloping behavior, especially in regimes where traditional analyses break down.

A significant strength of the proposal from Michigan State University was their unique expertise and capability to conduct Molecular Tagging Velocimetry (MTV). Standard quantitative flow visualization techniques (such as Particle Image/Tracking Velocimetry or PIV/PTV) require the introduction of tracer particles into the fluid and thus, careful calibration to ensure that the particles faithfully follow the flow. MTV uses a working fluid whose molecules fluoresce when exposed to laser light; this means that the tracers are guaranteed to faithfully follow the motion of the fluid. In addition, many of the typical problems in PIV/PTV techniques with near-wall measurements are a non-factor for MTV. The many advantages afforded by the application of this technique gave confidence to the ability of this effort to address questions that had long been difficult to answer.

After the research was underway, it was determined that certain portions of the flow regime would be better studied via three-dimensional quantitative flow visualization techniques. Dr. Munson recommended a DURIP award for a tomographic PIV system, which would allow the visualization of three-dimensional flow structures. One of MTV's limitations is that three-dimensional measurements are relatively difficult, so Tomographic-PIV is an attractive alternative. The equipment is also being utilized in active research funded by both the Office of Naval Research and the Air Force Office of Scientific Research.

Result

A number of scientific accomplishments have been already been achieved that expand knowledge of galloping dynamics for rectangular cylinders.

First, a static force measurement campaign was completed to characterize the importance of geometrical features (including aspect ratio, corner radius, and surface topology). Due to the small magnitude of the forces experienced by the cylinders, a custom force balance was developed to provide the required sensitivity and accuracy. The novel design of this force balance has recently been published in *Measurement Science and Technology,* and the geometry characterization is pending publication. Similarly to the force measurements, a custom torque sensor has been developed to characterize the moments in order to understand the stability to rotational galloping (Figure 1).

While the database of results generated so far is extensive, there appears to exist a previously unobserved critical change in behavior at a Reynolds number of 5,000 for sharp-cornered cylinders. (The Reynolds number describes the ratio of flow forces generated by the speed of the flow and the size of the body to the flow forces generated by viscosity or friction.) This transition in behavior appears to be driven by the behavior of flow separation from the corner and subsequent reattachment; when the reattachment point moves forward with increasing angle of attack, the cylinder will be stable to galloping. If reattachment never occurs, or if the reattachment point moves aft with increasing angle of attack, the cylinder will become unstable and susceptible to galloping. This is a stronger condition than had previously been understood; reattachment is necessary but not sufficient for galloping resistance. The behavior of the reattachment point is also critical in determining stability, since it directly influences the resultant forces on the cylinder.

Significant unsteady effects have also been discovered, which appear to grow stronger as the Reynolds number and oscillation amplitudes are reduced. This Reynolds number dependency indicates that, as friction plays a more dominant role in the dynamics, there is likely something fundamentally different in the nature of the boundary layer development that is leading to a substantial change in the loading experienced by the cylinder (Figure 2). The exact mechanisms are still under investigation.

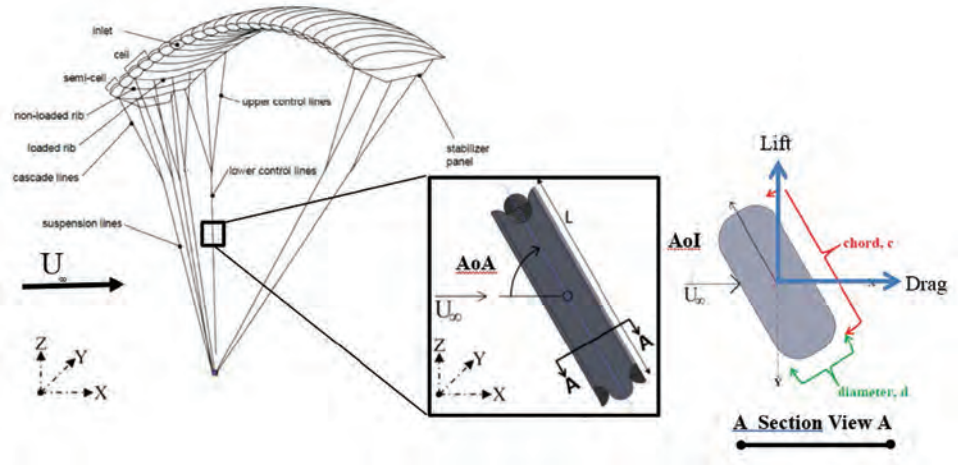


Figure 1: Parachute suspension line system. Angle of attack (AoA) and angle of incidence (AOI) are defined as in the figure. U∞ is the incoming free stream velocity.

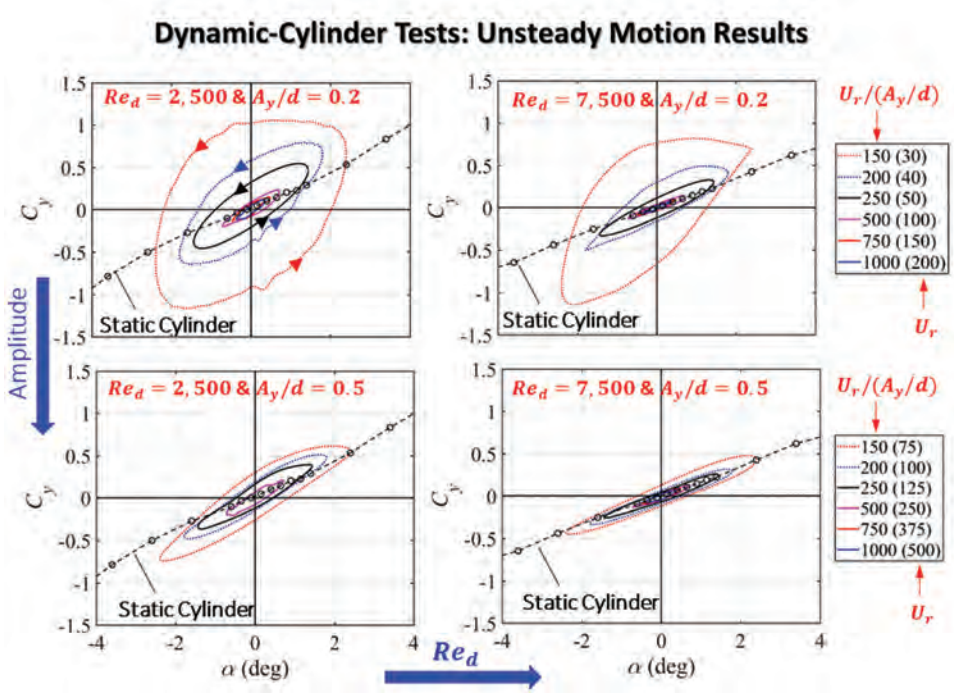


Figure 2: Dynamic cylinder behavior. For a given motion amplitude (denoted by A_y/d), decreasing the Reynolds number (Re_d) leads to an increase in dynamic motion, challenging the applicability of the quasi-steady assumption commonly used to analyze galloping behavior. Typically, the quasi-steady assumption has been used when values of $U_r/(A_y/d)$ are above 20. U_r is the reduced velocity of the incoming flow (velocity compared to the characteristic transverse velocity), A_y is the amplitude of the oscillation and *d* is the width of the cylinder.

Way Ahead

The investigation is still underway, with several objectives remaining to be completed. CCDC SC personnel have been engaged since the beginning of the effort and continue to remain involved in transferring the knowledge gained into other experiments. Potential exists for this work to inform future braided suspension line designs for next generation precision air drop systems. The results have also been used to inform complementary experiments currently ongoing at University of Massachusetts Lowell and the United States Air Force Academy.

SUCCESS STORY

Unmasking Phantom Yaw – Vortex Asymmetry on Slender Bodies at High Angle of Incidence

This ARO initiative resulted in **uncovering the fundamental mechanisms for vortex asymmetry on slender bodies**, which will allow control over the long-standing "phantom yaw" phenomenon. This discovery has potential to lead to enhanced flight control for projectiles, including the possibility of hyper-maneuverability.

This success supports these ARL Core Technical Competencies:

Ballistics Sciences

This success was made possible by the following ARO S&Es or Program Specialists:

- Dr. Matthew Munson, ARO Mechanical Sciences Division

Challenge

When slender bodies experience flight conditions where the angle of incidence exceeds a critical angle, the bodies often experiences a significant side force, whose direction and magnitude is unpredictable and, typically, undesirable. This side force, often referred to as "phantom yaw," has been long-known to result from breakdown of the symmetric production of vortices on the forebody; the causes (and cures) for this breakdown have been a topic of study for decades.

Phantom yaw is undesirable because it can often cause loss-of-control of a projectile; the side force experienced is simply not able to be counteracted by the available flight control mechanisms. Many strategies have been employed to control the vortex asymmetry, but the fundamental mechanisms for the initial symmetry breaking have received less attention.

Action

On a visit to Florida A&M University (co-located with Florida State University) in 2014, Dr. Munson met with Professor Rajan Kumar, who had studied the phantom yaw problem for a good portion of his career and had recently completed the construction of the FSU Polysonic Wind Tunnel Facility. Professor Kumar proposed an approach to tackling the fundamental flow physics questions that was not only compelling, but uniquely possible given the FSU/FAMU infrastructure and capabilities.

Dr. Munson encouraged Professor Kumar to submit a proposal to ARO for consideration. After review, Dr. Munson decided to support this effort on the hopes that not only would the fundamental mechanisms be uncovered, but that a new flight control strategy might be available. Elimination of phantom yaw is certainly important to ensure that projectiles can be adequately controlled; the potential to leverage phantom yaw to generate large forces, and thus large moments, is also particularly exciting.

In addition to the decision to support this research, Dr. Munson was able to secure significant resources from internal cost-matching opportunities since FAMU is a Historically Black College/University. Diagnostic instrumentation, including time-resolved quantitative flow visualization and pressure-sensitive paint, was also secured via the OSD HBCU/MSI Research and Education Program.

Result

Professor Kumar, through a carefully orchestrated experimental campaign, was

successfully able to identify the mechanism leading to symmetry breakdown. As the angle of incidence increases, the boundary layer forming on the surface of the forebody becomes more and more susceptible to perturbations. At some point a micro-imperfection (e.g. bump or divot) on the surface of the nose will generate a disturbance that will be amplified by the boundary layer, leading to the formation of a vortex that is different from the one forming on the other side of the body. Demonstrating that the "random" switching of the side force could be nearly eliminated by highly polishing the nose, he was then able to reintroduce perturbations of known size to "control" the initiation and degree of asymmetric force production. By systematically varying the size of the perturbation relative to the height of the local boundary layer, he was able to determine how to effectively "pin" the symmetry breakdown to a predictable location. This has the potential to make the side force controllable, by making sure that the "biggest" perturbation always occurs in a designed–rather than random–location (Figure 3). Thus, a flight controller could avoid phantom yaw or utilize it to make a rapid course adjustment.

In addition, the forebody vortices are known to interact with downstream control surfaces (such as tail fins), usually resulting in a degradation of control authority. Thus, control of forebody vortices could result in a much-desired capability to control this deleterious vortex wake system interaction. In this vein, Professor Kumar partnered with CCDC ARL WMRD researchers via a CRADA to study slender forebody vortex interactions with tail fins. A follow-on experimental campaign was recently funded via an OSD HBCU/MSI Research and Education Program and is underway.

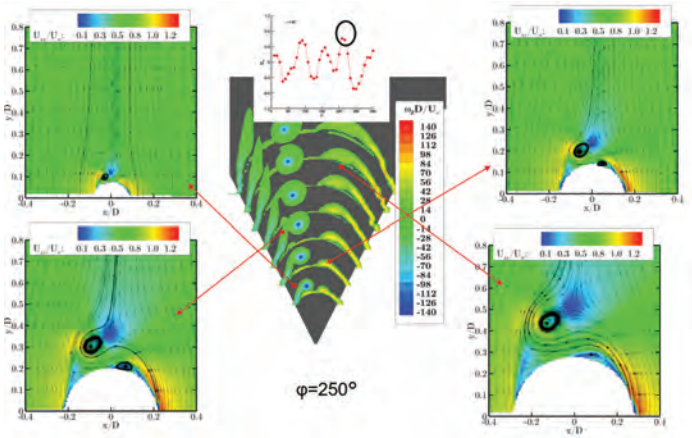


Figure 3: Asymmetric flow features at 40° angle of incidence and 250° roll angle. Strong vortex asymmetry can be seen (as evidenced by the contours of vorticity in the central panel), resulting in significant side load variations with roll angle (line plot).

Way Ahead

At a portfolio review hosted by Dr. Munson, Professor Ari Glezer of Georgia Institute of Technology was inspired by Professor Kumar's work to couple this forebody vortex control mechanism with an aft-body wake control strategy developed under a previous ARO grant award. This effort is aimed at providing a fundamental understanding of how the vortex forebody system and the aft wake interact to control forces and moments on slender bodies at high angles of incidence. This could provide the potential for spinless and/or finless projectiles. Early work has shown the ability to stabilize a slender body with no control surfaces through very small momentum injection near the junction between the nose and the cylindrical body.

CCDC ARL WMRD is also actively pursuing a new cooperative agreement with Professor Kumar to utilize his polysonic tunnel in order to provide experimental validation of their numerical simulations of advanced flight control methodologies for the Long-Range Distributed/Cooperative Engagement ERP.

Results

- Discovered fundamental mechanism of forebody vortex asymmetry
- Demonstrated control of side force production through engineered disturbances, thereby supporting the underlying mechanism and providing opportunity for generation of large forces/moments for control

Propulsion and Energetics Program

Current Scientific Objectives

01

Establish well-quantified mechanisms to predict ignition and initiation of energetic materials, especially undergoing thermal and physical insult; model and explain novel dynamics phenomena, including reaction mechanisms and electron-transfer rates to enable a deep understanding of chemical kinetics, thermochemistry, and catalysis, that in the long term will enable the design and synthesis of more effective propellants and explosives for the Soldier

02

Establish and quantify the key rate controlling processes (e.g. oxygen diffusion) in energetic materials that will enable the creation of future energetic materials that are safer for transport by the Soldier

03

Develop novel methodologies and approaches (beyond detailed chemical kinetics) to combustion modeling of heavy hydrocarbon fuels that will enable fully predictive large-scale modeling, thereby providing routes for the synthesis of future propellants that are more cost- and energy-efficient

04

Develop understanding of the reaction kinetics, chemistry and transport processes of combustion phenomena in heavy hydrocarbon fuels to enable predictive models at high pressures, especially for low-temperature ignition, providing the future Army with safer and more efficient propellants

Program Manager

Dr. Ralph Anthenien

Program Manager, Propulsion and Energetics Program
Chief, Mechanical Sciences Division
ARO Engineering Sciences Directorate

Dr. Anthenien completed his undergraduate studies at the University of California - Berkeley, receiving his B.S. in Mechanical Engineering in 1993. He received his Ph.D. from the University of California - Berkeley in Mechanical Engineering in 1998. He came to ARO in 2006 as the Program Manager for Propulsion and Energetics.

SUCCESS STORY

Enhancing Energetic Materials Performance through Surface Chemistry

This ARO effort has **identified key surface-chemical reactions that will enhance the overall reactivity of aluminum particles** that will allow safer, more powerful explosive and propellant formulations for the Army.

Challenge

Despite their high energy density, aluminum particles, like many other metallic propellant additives, are hampered by an inert oxide shell which both slows the energy release rate and lowers energy density. Activating or functionalizing this oxide surface using various schemes can increase reactivity and energy density; however, little is understood about the actual surface chemistry of these oxides or which hydroxyl species will best promote reactivity.

Action

Research in to combustion of reactive materials (nano-Aluminum and Teflon) in the mid-2000s revealed the discovery of exothermic surface chemistry that promotes energy transfer. This was originally shown to occur between the alumina surface layer on the aluminum particles and the fluorine from the flouropolymer based oxidizers. Dr. Anthenien encouraged further exploration of this phenomena, in particular extending this surface reaction with fluorine to other halogenated oxides such as iodine and chlorine. The exothermic surface chemistry was linked to improved reaction kinetics that enhances the overall combustion performance of the aluminized composite energetic material. Dr. Anthenien challenged Professor Michelle Pantoya of Texas Tech University to see if this effect could be further exploited, and she embarked on a new effort to improve the reactivity of micron scale Aluminum containing fuels through a careful study of the reactions at the interface of the alumina shell and the oxidizing agent. Dr. Anthenien also coordinated a seminar at CCDC ARL WMRD by Professor Pantoya to report on these initial results in October 2017. Researchers at CCDC ARL took interest and began coordinating further with Professor Pantoya. This resulted in a Director's External Collaboration Initiative between Dr. Chi-Chin Wu at CCDC ARL WMRD and Professor Pantoya being awarded in 2018. As part of this initiative, Professor Pantoya will continue to explore novel oxidative surface chemistry of metallic particles while Dr. Wu looks at plasma techniques to modify and tune the surface properties of the Aluminum particles.

Result

This work has sought several paths to harness greater power from Al combustion. One approach has been to chemically transform the Al2O3 passivation layer surrounding the Al core particle by exploiting surface reactions via a wet chemistry approach. As models for the surface layer of Al particles, ɣ-Al2O3 and ɣ-AlO(OH) nanoparticles were examined. Density functional theory calculations of dehydroxylation and dehydration energies predict that OH bridge bonds throughout ɣ-AlO(OH) require similar energy to

This success supports these ARL Core Technical Competencies:

Ballistics Sciences

Propulsion Sciences

This success was made possible by the following ARO S&Es or Program Specialists:

- Dr. Ralph Anthenien, ARO Mechanical Sciences Division

Results

- Established formal collaborative effort between CCDC ARL WMRD researchers and Texas Tech Researchers
- Texas Tech Graduate Student spent summer at CCDC ARL WMRD to aid in material characterization
- Demonstrated 30% improvement in detonation velocity of TNT with addition of treated aluminum particles

break compared with terminal OH groups abundant on the surface of ɣ-Al2O3 and are the most reactive sites. Experimentally, the predictions were confirmed by isolating representative surface reactions using ɣ-Al2O3 and ɣ-AlO(OH) nanoparticles suspended in an iodic acid solution to synthesize an oxidizing salt, aluminum iodate hexahydrate (AIH). PXRD and XPS identified species of whole materials and surfaces, respectively. The structural and compositional details were revealed by acquiring images, spectra, and determining component phase maps in the scanning mode via TEM. AIH formation from ɣ-AlO(OH) is linked to removal of OH bridge bonds and AIH formation does not appear localized on particle surfaces. These results link dehydroxylation and dehydration energies to reactions that produce AIH and provide a fundamental understanding of how to use hydration to control Al2O3 surface reactions and transform the reactivity of Al particles.

In conjunction with the ARL WMRD researchers, Professor Pantoya's research also explored mitigating the Al2O3 shell using different plasmas, leading to nAl particles with a thinner shell and different coatings, including carbon and AIH. The approach exploited a prototype atmospheric non-thermal plasma reactor with dielectric barrier discharge configuration for nanoparticle surface modifications. Plasma surface treatment of nAl is a novel "energy coupled to material" technique which alters the nAl surface properties without changing the bulk active Al core. Results indicated that Al2O3 shell can be mitigated with inert plasmas by as much as 40% using either helium (He) or argon (Ar). The particle surface becomes carbon-rich when treated with carbon monoxide (CO) / He plasmas. By immersing the plasma-treated nAl in an iodic acid (HIO3) solution, AIH crystals are formed on the nAl surface. Energetic tests utilizing laser-induced air shock for energetic materials (LASEM) show significantly enhanced energy release rates at the µs timescale for plasma treated nAl with AIH coating (Figure 1).

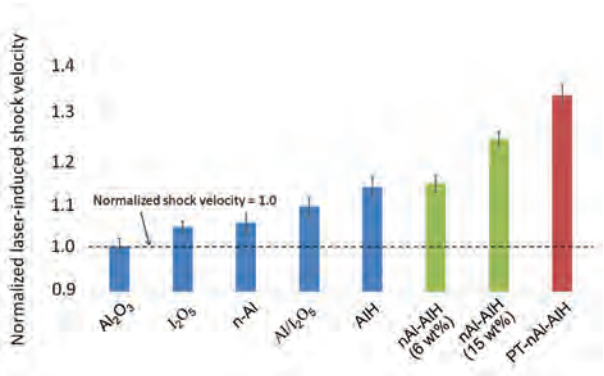


Figure 1: The laser-induced air shock velocities normalized to Al2O3 from the LASEM measurements at the microsecond timescale relevant to a detonation event.

Further, a graduate student from the laboratory of Professor Pantoya spent a summer embedded in the laboratory at CCDC ARL WMRD to complete the LASEM testing to characterize the treated particles and composite materials.

Way Ahead

In addition to being part of the formal collaborative effort, CCDC ARL WMRD researchers received samples of the novel materials as well as the treatment methodologies to continue to improve the technique and integrate the altered particles in to other formulations. The researchers at Texas Tech will continue their work, looking at other metallic such as Magnesium and Boron to see if similar enhancements through surface treatment, functionalization and activation can also be achieved with those metals.

SUCCESS STORY

Developing Novel Methods For Probing the Chemical Kinetics of Army Relevant Fuels

ARO funded research led to collaboration between ARL and academic researchers to **develop new diagnostic capabilities for the study of heavy hydrocarbon fuels** that will enable the design of more efficient engines.

This success supports these ARL Core Technical Competencies:

Propulsion Sciences

This success was made possible by the following ARO S&Es or Program Specialists:

- Dr. Ralph Anthenien, ARO Mechanical Sciences Division

Challenge

DoD directives for single fuel for the battle field (JP-8/Jet-A) are aimed at shortening the logistics tail for future forces. Unfortunately, this introduces reliability issues for current engines as there is currently no cetane number specification for jet fuel. It also increases complexity in "designing around" this requirement for future engines. Further, the future force will become more reliant on small engines for robotics and unmanned systems. These small engines are notoriously difficult to operate on heavy fuels and/or on diesel cycles due to their small size and concomitant high surface to volume ratio in the combustion chamber.

Action

The diversity of alternative fuel sources such as bio-oils and cellulosics has been growing significantly in the last decade. This is significant for the Army as while new feedstocks will be made to conform to JP-8 or F-24 jet fuel standards prior to acceptance, there is no cetane number standard for jet fuel. This creates the potential to adversely impact Army diesel cycle propulsion systems in their use of jet fuel under the single fuel for the battlefield policy. As the various feedstock produce final fuels that can chemically look very different from petroleum stocks despite passing the properties based jet fuel standard, Dr. Anthenien recognized that this could lead to significant variation in ignition characteristics. He advocated for investigations into the low temperature, high pressure ignition behavior of these fuels similar to what would be found in diesel cycle engines. In response to this call, in 2015 Professor Ken Brezinsky submitted a proposal to the Propulsion and Energetics program that combined the University of Illinois – Chicago (UIC) High Pressure Shock Tube and a unique 2-dimensional gas chromatograph (GCxGC). This would allow direct investigation of low temperature chemistry as well as high temperature combustion products in a way not previously possible. The proposal would investigate several fuels with alternative sources as well as conventional jet fuel. This work was then further enhanced by Dr. Anthenien via a Research and Education Program grant which was used to implement a time of flight mass spectrometer into the GCxGC system to allow for differentiation and identification of trace species in an complex chemical sample. This is key to developing quantitative knowledge of these low concentration species and using the information for the development of chemical kinetic models. Finally, working with Professor Brezinsky, Dr. Anthenien identified that a shortcoming of the facility was its test times. In 2019, a Research Instrumentation grant was awarded to further improve the facility by providing a driver extension on the shock tube lengthening test times to approximately

40 milliseconds (an approximately 5x increase over the previous facility) and bringing the systems capability fully in line with Army relevant ignition regimes. Recognizing both the uniqueness as well as the utility of the facility, CCDC ARL VTD expressed interest in collaborating with the UIC researchers to test other fuel types beyond what had been proposed originally. Dr. Anthenien proactively engaged ARL VTD leadership and UIC to develop an acceptable Joint Work Statement under a CRADA to allow the desired collaboration to move forward.

Results

- Formal collaborative effort between CCDC ARL VTD researchers and University of Illinois Chicago Researchers
- Unique facility developed to study, in-situ, trace levels of pre-ignition species in heavy hydrocarbon fuels
- Validation data of early time fuel-oxygenate compounds which are believed to control ignition behavior at low temperature and high pressure

Result

This work has developed a new facility for the study of hydrocarbon fuel ignition at diesel engine relevant temperatures, pressures, and residence times. Professor Brezinsky's team has already studied several fuels including an alcohol to jet (ATJ)/heptane mix, an ATJ/F-24 mix and pure F-24 at pressures up to 50bar for the facility's current capability of residence times of 7-8 milliseconds. The data has been compared to models of various types including lumped formation of characteristics intermediates (such as HyChem) and detailed mechanisms optimized for low temperature chemistry followed by a detailed high temperature premixed chemistry mechanism, such as the Lawrence Livermore National Laboratory (LLNL) type (Figure 2). The current chemical models do not properly capture the behavior of the sample fuel.

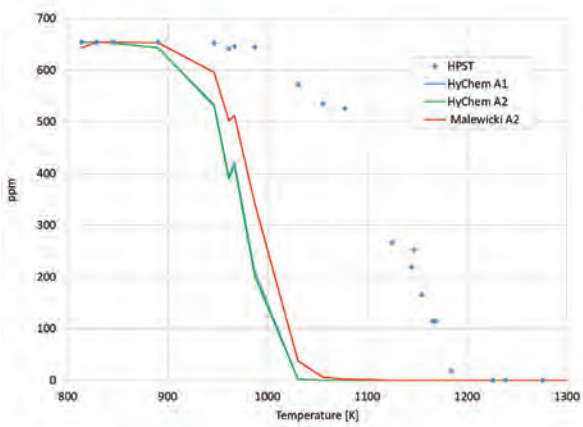


Figure 2: Comparison of several models (lines) against data (symbols) generated in the facility for undecene at various temperatures. Data is for 7ms residence times at an equivalence ratio of 0.93

The UIC researchers are continuing to work with researchers at Lawrence Livermore National Laboratories to use the data generated in the development of this effort to improve the chemical models so that the actual fuel behavior may be properly modeled. This will lead to improved engine design and resilience to off design fuels. Further, the researchers continue to collaborate with CCDC ARL VTD to develop an ignition model for operationally relevant fuels which will feed directly into research efforts under the CCDC ARL Versatile Tactical Power and Propulsion (VICTOR) Essential Research Program (ERP).

Way Ahead

The researchers will complete the implementation of the driver section extension lengthening the available residence time from 7-8 milliseconds up to 40 milliseconds. The focus of future studies will be on the detection of formaldehyde as it is predicted to be a significant early precursor for ignition, especially at low temperatures. The collaborative modeling effort with LLNL will continue as will the collaboration with VICTOR ERP researchers.

Solid Mechanics Program

Current Scientific Objectives

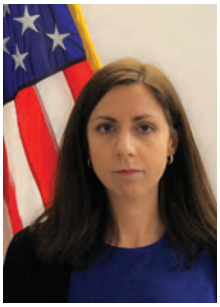
01

Uncover the physical processes responsible for deformation, damage initiation and propagation, and failure of material systems, which can lead to the creation of ultra-resilient, lightweight, and durable Soldier and system protections

02

Develop computationally efficient, robust, and predictive models, which can substantially reduce the time and cost required to develop new materials for future Army equipment

Program Manager



Dr. Denise Ford

Program Manager, Solid Mechanics
Mechanical Sciences Division
ARO Engineering Sciences Directorate

Dr. Ford completed her undergraduate studies at the University of Wisconsin - Madison, receiving her B.S. in Chemical Engineering in 2007. She trained as an engineer at Fermi National Accelerator Laboratory and Northwestern University, receiving her Ph.D. in Chemical Engineering 2013. She came to ARO in 2019 as the Program Manager for the Solid Mechanics Program.

SUCCESS STORY

Functionalizing Fiber Interfaces for Controlled Load Distribution

This ARO initiative resulted in **a method to grow nanowires at fiber interfaces** enabling lightweight materials to serve structural and protective functions.

Challenge

Equipment weight is a major burden on Soldier and system health and functionality. Materials that can carry high loads under static conditions typically fail under high strain rate conditions that result from impact and blast events. Weight can be reduced by combining structural and protective attributes into the same materials, therefore eliminating the need for an armor on top of a structural material. Composite materials are good candidates for this application because they can be designed for low weight

This success supports these ARL Core Technical Competencies:

Protection Sciences

Materials and Manufacturing Sciences

This success was made possible by the following ARO S&Es or Program Specialists:

- Dr. Denise Ford, ARO Mechanical Sciences Division
- Dr. Ralph Anthenien, ARO Mechanical Sciences Division

Results

- Developed synthesis process to create ZnO nanowire coatings on glass fibers
- Fibers delivered to ARL VTD collaborators Asha Hall and Latha Nataraj to test piezoelectricity as a damage indicator
- Patent filed for the process of coating fibers with ZnO nanoparticles
- Industry provided seed funding to evaluate the process for fiber reinforced nylon materials

and high specific strength, stiffness, and toughness; however, the interfaces between the parts of the composite are typically weak points in a structure.

Action

Professor Henry Sodano has been working to develop a method to grow ZnO nanowires on polymer fibers to strengthen the interfaces between fibers in a composite material. ARO program managers in Materials Science and Mechanical Sciences realized the value of his approach to Army systems, awarding Professor Sodano a STIR in 2012 to prove the concept. Professor Sodano developed his growth methods and composite designs to create a strong interface under static loading conditions that deliberately fails and transfers the load to the fibers when a high strain rate is applied. Different types of fibers – including polymer, carbon, glass, and aramid – are considered to tailor the composite's mechanical properties and weight. Recent studies supported by the Solid Mechanics Program under Dr. Anthenien focused on interfacial mechanics under various strain rates. The mechanics of the composite are tailored through the interaction of the ZnO nanowires with the fibers and matrix, and their microstructure within the interface between the fibers. ZnO nanowires were grown on carbon fibers embedded in a polymer matrix, nanowire thickness and length, thus morphology of interface, was varied. The stress distribution at the interface between the dissimilar materials was measured and the failure mechanisms were determined. Collaboration with Army researchers was also encouraged by Dr. Anthenien to further functionalize fibers for structural health monitoring, leading to a collaboration with Drs. Asha Hall Latha Nataraj at CCDC ARL VTD to develop composites which can indicate the level of damage to a structure based on the piezoelectricity of the fibers.

Result

Professor Sodano created a process for growing nanowires on fibers, which preserves the fiber strength during static loading conditions and allows the load to be transferred from the matrix to the fiber at high strain rate conditions. An example of ZnO nanowires grown on glass fibers is shown in Figure 1, along with evidence of successful load transfer at increasing strain rate. The ZnO interphase displayed up to 96% improvement in interfacial shear strength relative to untreated fibers at a quasi-static strain rate, which is caused by the creation of a functional gradient at the fiber-matrix interface due to the presence of the nanowires. A 68% decrease in interfacial shear strength was observed at rates greater than 2000 s-1, due to matrix stiffening, and resulting in brittle fracture of the ceramic interphase. Different morphologies of the nanowires were shown to effect the strengthening of the interfaces and the distribution of the load at different strain rates. Tests of tensile properties were measured before and after nanowire growth, revealing an 8.8% increase in the elastic modulus and a 13.2% increase in the tensile strength of an aramid fabric with a ZnO nanowire interface over the neat fabric. The aramid fabrics were also subjected to impact testing, showing a 20% increase in the v50 impact performance for the fabric with ZnO nanowires at the interface over the neat fabric. Professor Sodano has further explored the growth of ZnO nanowires and nanoparticles on various types of fibers, providing a path forward for tailoring the strength and weight of composite materials for future Army systems.

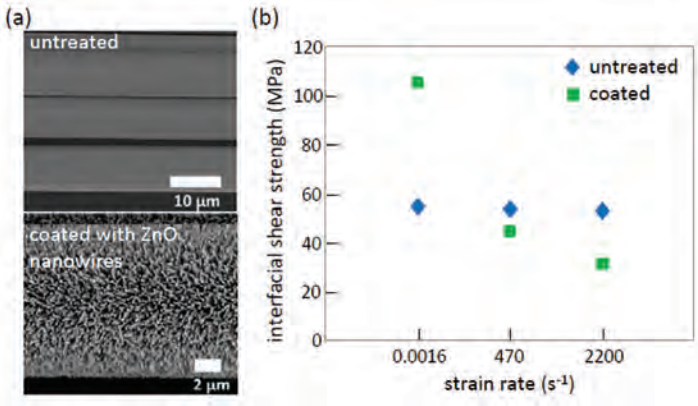


Figure 1: ZnO nanowires (a) grown on the surface of glass fibers and (b) interfacial shear strength vs. strain rate of glass fibers.

Way Ahead

Now that the relationship between interface morphology and strength has been revealed and processes have been developed for tailoring the growth of nanowires to achieve desired morphologies, the processes must be scaled for application in practical composite materials. The mechanisms of failure at interfaces remain unclear, with studies underway in collaboration with CCDC ARL.

SUCCESS STORY

Predicting The Deformation Behavior of Ultrahard Lightweight Ceramics

ARO funded research created a **predictive model for the ballistic resistance of boron-rich ceramics**, that may open the door to new protective materials.

Challenge

Boron based ceramics are superhard, strong, and lightweight, but fail under ballistic loading. The atomic structure of superhard boron-rich solids collapses and amorphisizes under high pressure loads, and these amorphous regions nucleate cracks. Boron carbides and boron oxides have cage structures, which can be doped or morphologically tailored to prevent amorphization. These complex deformations create significant challenges to screening and evaluating enhanced structures and compositions.

Action

Professor Ghatu Subhash of the University of Flordia was selected by ARO to receive a DURIP in 2016, which provided funds to upgrade his Raman spectrometer, essential to a unique method that he was developing to characterize the deformation behavior of boron carbide. The method successfully combines density functional theory, density functional perturbation theory and Raman spectroscopy to predict the amorphization of boron carbide polymorphs, thus providing direction for tailoring the structures to resist amorphization. Solid Mechanics Program Manager Dr. Ralph Anthenien realized that this approach could be extended to other materials that may have greater potential than boron carbides in protection systems. One such material is boron suboxide, which has

This success supports these ARL Core Technical Competencies:

Protection Sciences

Materials and Manufacturing Sciences

This success was made possible by the following ARO S&Es or Program Specialists:

- Dr. Denise Ford, ARO Mechanical Sciences Division
- Dr. Ralph Anthenien, ARO Mechanical Sciences Division

Results

- ARO funded researchers collaborating with Satapathy Sikhanda at ARL WMRD to develop a predictive penetration model for ceramics
- ARL and academic collaborative research was published in the *International Journal of Impact Engineering*
- Identified relevant physics of amorphization under severe loading conditions

higher theoretical hardness and compressive strength, and an atomic structure that is more resistant to bending than boron carbide. Boron suboxide is also highly prone to twinning at the nanoscale, which may increase tensile strength, microhardness, and fracture toughness in structural ceramics. Thus, in 2017 Professor Subhash received an award to study the amorphization of twinned vs. untwinned boron suboxides using his previously developed technique combining Raman spectroscopy and quantum mechanical calculations. He has continued to progress with creating a predictive model for the high-pressure deformation of boron-rich solids by adding TEM and computational spectroscopy characterization, and was also encouraged by Dr. Anthenien to establish a collaboration with Satapathy Sikhanda at CCDC ARL WMRD.

Result

This effort has connected atomic structure to ballistic performance of boron-based ceramics and provided a new predictive penetration model for brittle materials, which includes the effects of amorphization on boron carbide. New spherical formulations used throughout the model decrease solution complexity and increase internal consistency in the model. Universal constants used in the constituent model allow it to be applied to a variety of brittle materials without the need for experimental data on both intact and damaged materials as inputs (Figure 2). Progress has also been made on understanding the formation of nanotwins in structural ceramics and their influence on deformation. SEM analysis showed flower-like particles in B6O power, which was confirmed by TEM to be evidence of extensive nanotwinning. Sintering attempts for characterization of the powder were partially successful, and further work is being conducted to understand the effects of processing parameters on the density of the powder.

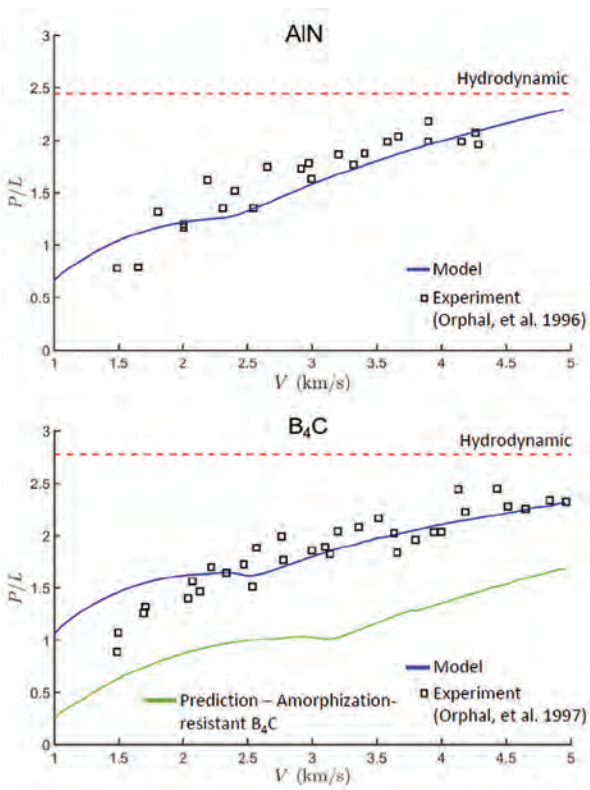


Figure 2: Normalized depth of penetration vs. impact velocity for a long tungsten projectile impacting structural ceramics.

Way Ahead

Continued investigation is required to understand the effects of nanotwins on the properties of boron suboxides. Investigations of the microstructure, composition, bulk elastic properties, hardness, and compressive strength will be conducted. Molecular dynamics simulations will also be performed to provide information about the effects of the atomic scale structures on the shock-response of boron-rich solids. A more complete understanding of the structural effects of boron-rich solids on their properties and performance, as well as how to realize the theoretical properties of the materials will help identify new compositions, and ultimately better materials to protect the Soldier and materiel.

Earth Materials and Processes Program

Current Scientific Objectives

01

Determine how grain-scale features influence bulk properties in unconsolidated earth materials, to enable rapid and accurate simulation of vehicle terrain interaction.

02

Develop methods to remotely determine earth surface properties, to enable unmanned reconnaissance to inform routing decisions or tracking enemy movements.

03

Enable prediction of earth surface interaction with air and water at Warfighter-relevant spatio-temporal scales (microns to 100s of kilometers), that may provide advance notice of environmental hazards ranging from contaminant dispersal in dense urban environments to brownout in arid regions.

Program Manager

Dr. Julia Barzyk

Program Manager, Earth Materials and Processes

Mechanical Sciences Division

ARO Engineering Sciences Directorate

Dr. Barzyk completed her undergraduate studies at the University of Rochester, receiving her B.A. in Geology in 1998. She received an M.S. in Geological Sciences from the University of Florida in 2000 and an M.S. in Environmental Science and Policy from the University of Chicago in 2002. She received her Ph.D. in Geophysical Sciences from the University of Chicago in 2007. She came to ARO in 2015 as the Program Manager for the Earth Materials and Processes Program.

SUCCESS STORY

Imaging The Physical Controls On Rock Debris Surface Properties With A Novel 3D Reconstruction Method

This ARO funded effort resulted in a **new method to determine earth surface properties over large areas,** enabling the mapping and characterization of deposit characteristics down to centimeter levels.

This success supports these ARL Core Technical Competencies:

Network and Information Sciences

Computational Sciences

This success was made possible by the following ARO S&Es or Program Specialists:

- Dr. Julia Barzyk, ARO Mechanical Sciences Division

Challenge

Bouldery talus fields, deposits of boulders and other debris created by rockfall from cliffs or steep slopes, are rugged environments with large void spaces within them, which can provide animal habitat and ample cover or shelter for people. The presence of talus affects the trajectories of further rockfall and other bouncing objects. Talus can alter hydrology and affect the chemistry and water quality of runoff, affecting planning for spill mitigation and waste disposal. Some talus fields locally maintain unusual cold temperatures, with implications for interpreting terrain based on thermal imaging. Talus fields affect patterns of vegetation, commonly appearing in aerial or satellite imagery as clear areas in vegetated terrain, but often the end of the talus slopes is obscured in forest. In addition, the deposits are the best record of past rockfall, which allows a critical assessment of rockfall hazards in habitated settings.

Unfortunately, the formation of talus has been poorly understood due to the inability to determine the relative effects of dynamical processes (i.e., fracturing and sorting of rocks as they travel downslope during rockfall events) and post-depositional processes (i.e., the action of weathering and erosion processes that redistribute, sort, and break down deposited rockfall debris over time) in controlling talus grain size and sorting, due largely to the difficulty of collecting data on changes in rock debris surface properties at sufficient spatial and temporal scales.

Action

In 2014, Dr. Barzyk began discussions with Professor Dylan Ward at the University of Cincinnati on his idea that photogrammetry could be used in conjunction with a method of determining the exposure ages of rocks termed cosmogonic nuclide dating to investigate controls on talus formation. While the proposed effort clearly had relevance to the geoscience community, Dr. Barzyk reached out to Mr. Michael Lewis at the U.S. Army Corps of Engineers Engineer Research and Development Center Geospatial Research Laboratory (ERDC-GRL) to determine how the research could be targeted towards highest Army impact. Through discussion with Mr. Lewis, it was determined that the research could have high relevance to dismounted routing in mountain environments as Solider energy expenditure is very high when moving through talus. Dr. Barzyk worked with Professor Ward to help address a number of concerns raised by ERDC-GRL regarding the need to account for a range of rock types and to develop a model that could be useful with only a very general knowledge of local geology, thereby improving the research plan.

Result

To test the relative roles of the dynamical and post-depositional processes in controlling talus grain size and sorting, this study took advantage of a distinctive field site: a 20-km-long escarpment that varies continuously in height along its length, where rockfall is sourced from similar rocks, and where it is also possible to identify and quantify a range of deposit ages (Figure 1). The central task was to generate high-resolution (sub-meter) digital topography and co-registered true-color imagery over the study area using structure-from-motion photogrammetry and to use these products to classify surface types and debris size distributions. Cosmogonic exposure-age dating of large talus boulders and bedrock exposed during cliff retreat constrains debris longevity and rates of production, and field measurements of talus boulder compressive (impact) strength,

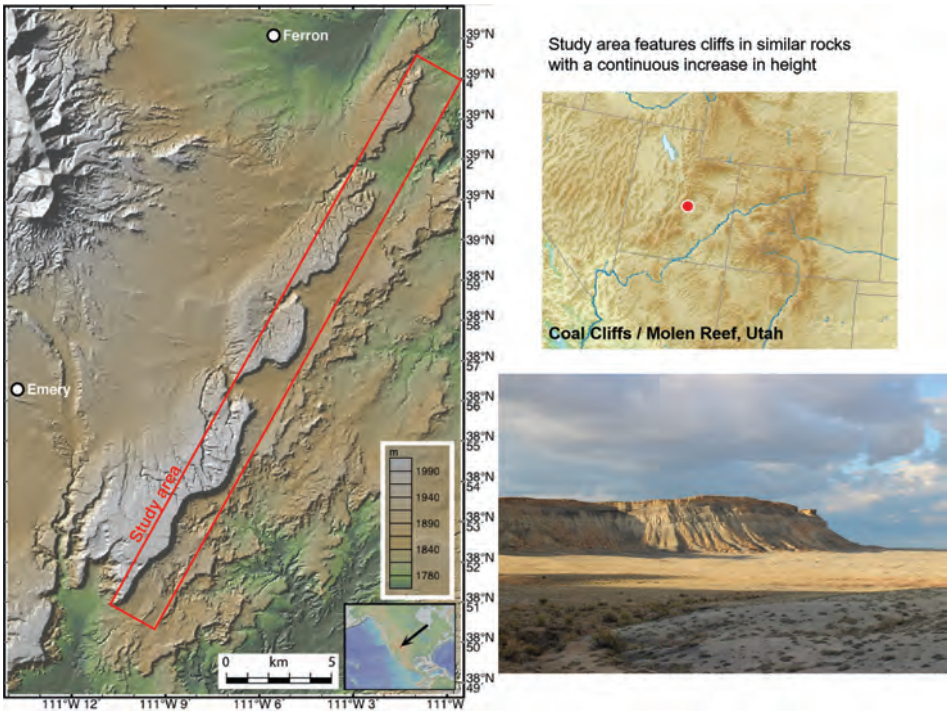


Figure 1: Field study area, Coal Cliffs / Molen Reef, Utah.

microfractures, and pitting help reveal processes and rates of postdepositional processes. The scientific goals for this project fell into two categories. The primary focus was understanding the controls on development of talus fields and their properties, as described above. A second, broader question was to relate these properties to longer-term landscape evolution, as the coarse sediment alters hydrology and can inhibit erosion of the footslope below cliffs.

To address these questions at field scale required surveying characteristics of rockfall deposits over a large geographic extent, to determine how they vary with natural variability, for example, in the height of the escarpments, and an understanding the age and residence time of the deposits, to determine how weathering alters the deposits. High-resolution digital topography was required to extract the grain size distributions, better than the meter-scale resolution of typical airborne LIDAR scans, but covering similarly large areas. Therefore, a method with the ability to measure these properties at high resolution across a wide enough area was required and developed (Figure 2).

From analysis of the data, it was determined that stream incision and shallow landsliding were primarily responsible for distributing talus and that the reworking of these deposits is episodic but much more frequent than the generation of new rockfall. Professor Ward was successful in developing tools for working with images from a range of sources including ground-based handheld photos, unmanned aerial vehicle (UAV) video frames, and georeferenced UAV photographs. The georeferenced UAV photographs resulted in the best topographic reconstructions, but the other sources of imagery proved to be sufficient for the analyses and may be more expedient under certain circumstances. Professor Ward also developed software tools to map grain size distribution of the talus deposits at broad spatial scale and high resolution. These results have been published in two high-impact journals, *Earth Surface Processes* and *Landforms and Lithosphere*.

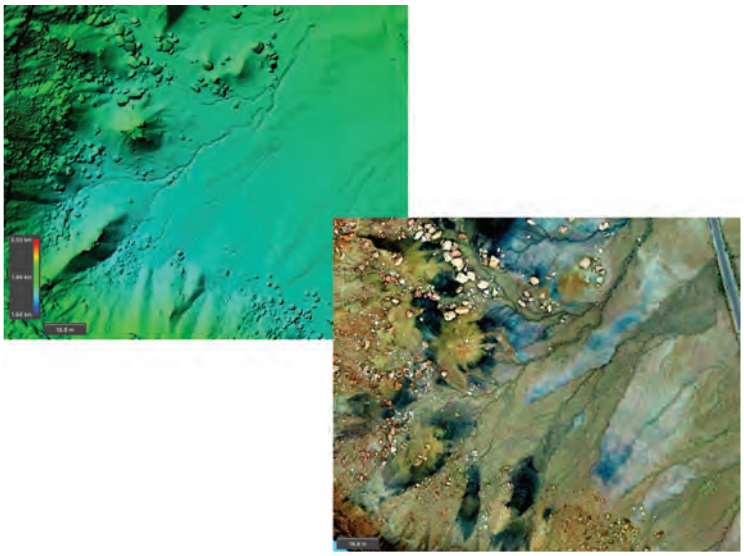


Figure 2: Photogrammetric reconstructions resolve topography to 5 cm / pixel and highlight multiple generations of talus of a range of sizes. Light-colored boulders have been more recently reworked to a lower elevation.

Results

- Identified previously unknown mechanisms responsible for creating surface features of relevance to mobility in mountainous terrain
- Developed software tools to perform topographic reconstructions from handheld and UAV photos
- Publications in two high-impact journals

Way Ahead

This structure-from-motion photogrammetry approach was developed using inexpensive consumer UAVs, robust libraries for computational image analysis, and geological surface exposure dating methods. To take advantage of these new methods, this project combined them in a novel way in a carefully chosen field area. Following this effort, there is significant opportunity to use this combination of tools in other landscapes or fundamental and applied research.

Professor Ward plans to extend this work to work towards understanding the processes by which talus is redistributed in a desert environment through development of a process-based model of how the duration and intensity of precipitation events result in specific, rapid erosional responses, given the interaction of surface materials (shale bedrock and sandstone talus) with moisture. He is also planning a visit to ERDC-GRL in 2020 to present a seminar on his research and hold meetings with ERDC-GRL staff to explore how this work may further impact dismounted routing tools and the development of software to use photographs and video generated at low cost to develop high-resolution 3D topography for change detection.

SUCCESS STORY

Dust Modeling To Mitigate Hazards

Through detailed field measurements, this research has **overturned long-held assumptions about the relationship between wind speed and particle emission** that will be used in Army atmospheric models to improve predictions of brownout events.

Challenge

The relationships between the occurrence of sand transport and dust aerosol emission, wind speed and soil moisture have not been well constrained due to the difficulty of collecting high-frequency particle emission and wind speed data in the field environment, and therefore how particle emission scales with increasing wind speed had not be determined.

Action

In 2014, Dr. Barzyk initiated conversations with Professor Jasper Kok at the University of California - Los Angeles (UCLA) regarding his proposed research effort on the relationship between the movement of sand grains through saltation (a 'jumping' process by which a grain that is lifted from the surface falls back to the surface impacting and ejecting another grain from the surface). Dr. Barzyk encouraged the researchers to submit a proposal, and enabled Ms. Sandra LeGrand at U.S. Army Corps of Engineer Research and Development Center Cold Regions Research and Engineering Laboratory (ERDC-CRREL) to provide feedback. As the research was underway in 2016, Dr. Barzyk initiated a site visit with Ms. LeGrand to UCLA to meet with Professor Kok and his co-PI Professor Gregory Okin. Through this meeting Ms. LeGrand provided information on Army needs in dust modeling, which are related to hazards associated with Degraded Visual Environment and abrasion. Conversations were also started on additional analyses that could be performed to provide direct support to ERDC-CRREL. Dr. Barzyk initiated an additional meeting in June 2019 at New Mexico State University, one of the locations for field studies conducted in the effort, to begin discussions on developing research needs, especially as related to a DURIP awarded to Professor Okin in 2018.

Result

The UCLA team has used extensive field experiments to show that the trajectories of blown-sand particles surprisingly stay approximately constant with increasing wind speed (Figure 3). This seemingly counterintuitive result implies that the sand flux simply scales linearly with the wind shear stress, which was confirmed through direct measurements of the sand flux at three different field sites (Figure 4). This result represents a paradigm shift: the widely-used nonlinear saltation flux laws that this work overturns originated with the pioneering work of Ralph Bagnold, widely considered the founder of aeolian science, in the 1930s. This result was recently published in the high-impact journal *Science Advances.*

Figure 3: Field measurements of particle emission and wind speed.

The team has tested whether different particle sizes in a soil have different threshold wind speeds above which they become mobile. The prevailing wisdom has been that different-sized particles in a given soil become mobile at different wind speeds. In other words, sand transport and dust emission parameterization in most large-scale models assume that sand transport is governed by "size-selective susceptibility", with larger particles requiring greater wind speed. The UCLA team showed that this is not the case, and that there is only a single initiation threshold for the entire soil ("equal susceptibility") (Figure 5). This important insight is easy to implement in dust emission modules and thus can improve dust simulations in large-scale models.

A long-standing challenge in the physics of wind-blown sand and dust transport is that it is driven by turbulent winds, and thus is often highly intermittent. In contrast, existing models and parameterizations describe sand and dust transport as a process that is uniform in time and space, and driven by a constant wind speed. This clear disconnect between theory and models on the one hand, and the reality in the field on the other,

This success supports these ARL Core Technical Competencies:

- Network and Information Sciences
- Computational Sciences

This success was made possible by the following ARO S&Es or Program Specialists:

- Dr. Julia Barzyk, ARO Mechanical Sciences Division

Results

- Developed new paradigm to relate wind-blown particle transport to wind speed
- Results led to contract awarded by the U.S Army Engineering Research and Development Center-Cold Regions Research and Engineering Laboratory to UCLA researchers to use the resultant data set to improve dust transport prediction using numerical models of the atmosphere for both weather and climate applications
- Article publication in high-impact journals including *Science Advances*

is likely one of the main causes of the poor performance of parameterizations of sand transport and dust emission. Building on their extensive data set, the team has developed a straightforward parameterization for sand transport that accounts for the effects of intermittency. They have shown that the explanatory variable is the fraction of time that sand transport is occurring and have obtained a simple parameterization for this that can be readily implemented into large-scale models. In 2018, a contract was awarded by ERDC-CRREL to the UCLA team to use the resultant data set to improve dust transport prediction on shorter timescales through incorporation into Army's operational atmospheric model, the Met Office's Unified Model.

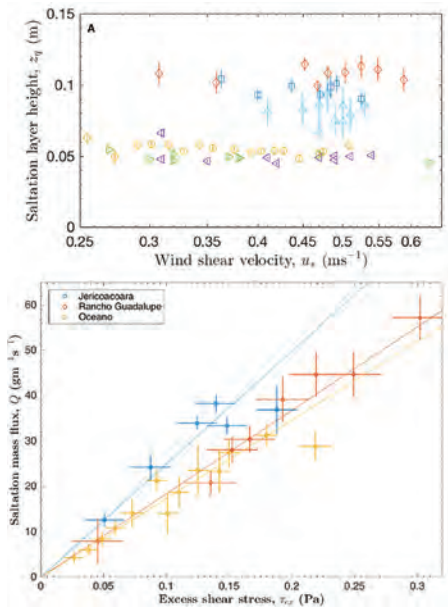


Figure 4: Wind-blown sand flux scales linearly with wind stress.

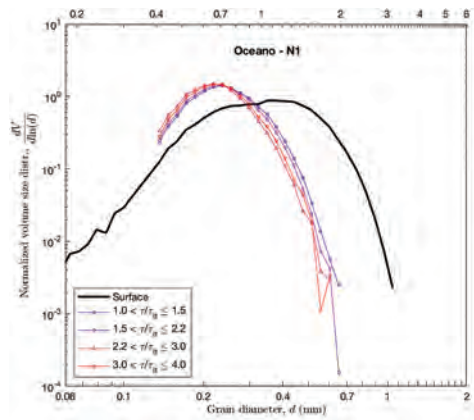


Figure 5: A soil with mixed particles has a single threshold wind speed for transport initiation.

Way Ahead

A DURIP was awarded in 2018 to Professor Gregory Okin of UCLA to build a wind tunnel that will be the first of its kind in that will be both field deployable and climate controlled. The equipment will fill a significant gap in data collection on wind-blown particles, as currently measurements are made in laboratory wind tunnels, in which climate control is possible, or in field-deployable wind tunnels, in which climate control has not been possible. The UCLA team has initiated work on the ERDC-CRREL contract to improve predictions of dust emission and transport, and discussions have begun with CCDC ARL CISD researchers about potential access to ARL's Meteorological Sensor Array, a suite of towers designed to measure wind speed and meteorological data in a topographically complex environment located at the USDA Jornada Experimental Range.

Computational Architecture and Visualization Program

Current Scientific Objectives

01

Create interactive yet accurate/realistic visualizations/simulations through new theory, and analysis of hybrid and acceleration techniques that combine the accuracy of numerics, with the speed of computer graphics. If successful, it is anticipated to lead to enhanced training capabilities for more effective combat readiness.

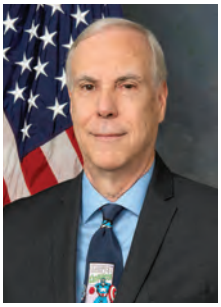
02

Create new, energy efficient techniques and architectures for the optimal realization of multi-core systems, and future hybrid and exascale systems, to process and operate in resource constrained environments. This will support complex, resource-demanding, real-time battlefield applications.

03

Devise scalable and communication efficient algorithms to effectively handle the volume, heterogeneity, and multi-modality of complex data arising from emerging and future Army applications for real-time, accurate delivery and analysis of critical Army data, to all necessary and relevant combat units.

Program Manager



Dr. Mike Coyle

Program Manager, Computational Architectures and Visualization
Computing Sciences Division
ARO Information Sciences Directorate

Dr. Coyle completed his undergraduate studies at Boston College, receiving his B.A. in mathematics in 1976. He trained as an applied mathematician at Rensselaer Polytechnic Institute, receiving his Ph.D. in mathematics in 1990. He began working for the Army as a mathematician in 1984. He came to ARO in 1999 as the Program Manager for what was then called the Discrete Mathematics and Computer Science Program.

Information
Sciences
Directoriate

- **Computing Sciences Division**
- Mathematical Sciences Division
- Network Sciences Division
- Technology Integration & Outreach Division
- ARO Special Programs

This success supports these ARL Core Technical Competencies:

Network and Information Sciences

Computational Sciences

This success was made possible by the following ARO S&Es:

- Dr. J. Michael Coyle, ARO Computing Sciences Division

SUCCESS STORY

Transforming 3D Reconnaissance Data into Geospatial Intelligence

An ARO supported Phase I Small Business Innovation Research (SBIR) project has **implemented a real-time, GPS free navigation technique that was successfully field tested.**

Challenge

Current Army, Department of Defense, and civilian capabilities for site exploration missions in urban-suburban areas, especially reconnaissance and rescue operations, are inaccurate, heavy, expensive, dangerous, and time consuming. Unmanned Aerial Systems (UAS) could potentially provide real-time military reconnaissance, fire and rescue, law enforcement, and other first-responders with important new ways to enhance mission effectiveness and reduce operational costs. While the small Unmanned Aerial Vehicles needed for such missions are now available at reasonable cost, the navigational and control systems and associated software required to conduct such coordinated, precision autonomous operations in low altitude urban and suburban airspaces, are not yet available. This is because current state-of-the-art systems rely heavily on the U.S. NAVSTAR global positioning system (GPS) and global navigation satellite system (GNSS). However, in low altitude urban and suburban airspaces, the high density of obstacles and the presence of people necessitate a degree of navigational precision and reliability that cannot be met by GPS, which can have limited precision near buildings, or existing "sense and avoid" technologies (e.g., The Traffic Alert and Collision Avoidance System (TCAS), which has been widely deployed in manned aircraft). Software tools and algorithmic techniques not dependent on GPS are necessary for UAS navigation in the urban-suburban airspace.

One such technique is three dimensional (3D) map-matching. 3D map-matching is a navigational basis that is orthogonal to radio navigation and consequently does not suffer from the same limitations and vulnerabilities of GPS. Early 2.5D map matching systems such as Terrain Contour Matching (TERCOM), were effectively employed in cruise missile navigation prior to GPS. The ability to pre-acquire detailed 3D geospatial data has increased exponentially since the time of TERCOM. Moreover, commodity sensors are now available which generate real-time point-clouds that could potentially be matched to the pre-acquired 3D geospatial data to provide rapid, precise localization in many GPS denied environments.

However, two problems have slowed the evolution of efficient 3D map-match solutions. First, because 3D geospatial data sets are so large, it can be difficult to transmit and maintain them over bandwidth and latency constrained networks using conventional data delivery approaches. Second, the processing of these massive 3D datasets by 3D map-matching algorithms can be very inefficient because the matching algorithm is typically forced to process a large amount of occluded data that is irrelevant to the immediate 3D map-match localization solution. This is especially true in densely occluded natural terrains or within the urban canyon.

Action

This ARO PM was approached by researchers/representatives from a small company located on the Centennial Campus of North Carolina State University. These researchers

were interested in support regarding their efforts in the area of GPS denied navigation in urban environments. This is an area of great interest to the Army and DoD and the ARO PM felt support was highly warranted. After discussions with a computational scientist from the then ARL Survivability and Lethality Analysis Directorate (SLAD), who had vast experience in modeling and analyzing urban environments, it was decided that an SBIR award would be the most appropriate approach. The ARO PM wrote and submitted an SBIR topic entitled, "Transforming 3D Reconnaissance Data into Geospatial Intelligence." The objective of the topic was to design, analyze, and implement new algorithms and a software system for streaming and processing 3D reconnaissance data for enabling large-scale UAS operations in the low altitude urban-suburban airspace. The topic was selected for funding and two Phase I grants were awarded to Opto-Knowledge Systems, Inc, (OKSI) a small California company, and to Primal Systems, Inc., a small North Carolina company. In the course of the Phase I effort, the ARO PM invited representatives from ARL West to review meetings and live demos held and performed at the OKSI office complex. ARL West has expressed great interest in the work and both ARL West and OKSI has a great desire to establish a Cooperative Research and Development Agreement (CRADA), especially after receiving the news that OKSI has been awarded a Phase II grant.

Result

OKSI supported by an ARO Phase I SBIR grant demonstrated a proof-of-concept for all of the key elements of GPS denied navigation capability, including a demonstration of octree compression, streaming over a network, multiple UAS streaming to and from a server, and GPS-denied navigation from a 3D map in real-time. Specifically, during the Phase I effort they implemented an octree representation in global world coordinates and demonstrated a 99.9% lossless reduction in 3D data storage / streaming requirements. OKSI then implemented a baseline database, a Neural Autonomic Transport System (NATS), an open source messaging system, data server, and streamed maps and measurements from the ground control station to the UAS platforms over a 4G-LTE cellular network. They implemented 3D Navigation in real-time on UASs and flew a set of two UAS platforms concurrently (Figure 1), performing real-time mapping to the server and open-loop navigation on-the-fly. This resulted in a proof-of-concept for the proposed GPS denied navigation capabilities, eliminating most of the technical risks associated with a Phase II effort. OKSI completed all of the objectives of the Phase I effort and exceeded expectations by demonstrating all of the above capabilities (e.g., 99.9% data compression, real-time streaming, GPS-denied navigation) on two platforms, in-flight, concurrently. Their success from the Phase I effort paves the way for the successful development of a prototype system and subsequent commercialization during the Phase II effort and beyond.

Figure 1: UAS in-flight (left) as a part of a two UAS joint 3D octree mapping and navigation mission. Example 3D octree map and UAS locations in real-time during this experiment (right).

Results

- Presentation of SBIR Phase I results at the Military Sensing Symposium (MSS)
- SBIR Phase II grant awarded to pursue integration into navigation systems
- Establishment of a CRADA with ARL West in progress for integration and testing of the GPS-independent navigation capabilities

Way Ahead

A SBIR Phase II award has been made to OKSI who will continue to partner with ARL West, including the establishment of a CRADA, with the goal to transition their system to DoD's Tiger Shark UAS program for integration and testing of the GPS-independent navigation capabilities.

SUCCESS STORY

High-Performance Static and Streaming Tensor Factorization Algorithm

ARO supported researchers **developed an algorithm called CPstream that enhances the speed of data streaming**, with anticipated future impacts to Army mission command centers, Army High Performance Computing centers, and Army machine learning applications.

This success supports these ARL Core Technical Competencies:

Network and Information Sciences

Computational Sciences

This success was made possible by the following ARO S&Es:

- Dr. J. Michael Coyle, ARO Computing Sciences Division

Challenge

Computations involving unstructured and irregular memory accesses, as well as data-dependent and problem instance specific task dependencies have always represented important, but challenging classes of problems for high-performance computing. One such emerging class of problems is techniques for tensor factorization. These techniques are widely used for dimensionality reduction and clustering in machine learning, latent parameter estimation and source separation in signal processing, and numerous other applications in diverse disciplines, such as cyber-security, chemistry, and psychology. Tensors are used to model multi-way interactions and are a generalization of matrices to higher dimensions (modes). The size of the datasets that need to be analyzed using tensor decompositions is already measured in several gigabytes or terabytes, and it is expected to grow as different types of data are collectively analyzed and new application areas for tensor analysis emerge.

Though there exist some widely used software packages (e.g., n-way toolbox, Tensor Toolbox, and tensorlab), they are not optimized for the efficient processing of large, sparse, and irregular tensors. They cannot handle tensors with many modes; and cannot take advantage of current and emerging high-performance computing architectures. In addition, though there has been extensive research on how to efficiently operate on unstructured and irregular sparse matrices, the nature of the computations that underlie many of the tensor factorization algorithms create numerous challenges associated with efficient tensor storage schemes; reducing the required number of operations and amount of required intermediate memory; organizing the computations to take advantage of deep memory hierarchies; and extracting, synchronizing, and load-balancing their parallel execution. Developing high-performance and scalable parallel formulations for the different types of tensor decompositions and underlying optimization algorithms for static and streaming tensors on current and future (parallel) computing architectures, and making them available in an easy-to-use open source software tool will significantly enhance the ability to analyze very large multi-way data.

Action

In response to the above scientific challenge, and the Army's interest in high performance computing, machine learning, and source separation in signal processing, and after discussions with and recommendations from Army computer scientists from ARL Computing and Information Sciences Directorate, this ARO PM recruited Professor George Karypis of the University of Minnesota. Professor Karypis is a world renowned researcher and expert in high performance and parallel computing, computational load balancing, and data mining. This researcher also has vast experience in interacting with the Army and ARL from being a former top researcher for the Army's High Performance Computing Research Center, and a former ARL Technical Assessment Board member. Professor Karypis was asked to develop new theory, algorithms, and data structures for fast and efficient serial tensor factorization, in addition to scalable high-performance parallel algorithms and open source software tools for tensor factorization on shared-memory, distributed-memory, and emerging parallel architectures. Such research could significantly reduce the computational effort associated with tensor factorization, which is now broadly used in many science and engineering disciplines. In addition, the proposed development and release of the high performance tensor factorization software tool will enable researchers and practitioners to analyze larger datasets. Furthermore, the high performance computing insights that this project will generate for emerging programming models and architecture will be applicable to many other types of problems that involve unstructured and irregular computations for both the military and civilian domains.

Result

In many applications, a tensor's entries arrive in a streaming fashion for a potentially unbounded amount of time. Existing approaches for streaming sparse tensors are not practical for unbounded streaming because they rely on maintaining the full factorization of the data, which grows linearly with time. The goal of this research effort was to come up with effective streaming tensor factorization algorithms that work well with sparse streaming ('infinite') data without memory/complexity explosion. To this end, they developed CPstream, an algorithm for streaming factorization in the model of the canonical polyadic decomposition, a mathematical technique for expressing a high dimensional tensor as a linear combination of very low dimensional tensors, which does not grow linearly in time or space, thus practical for long-term streaming. CPstream incorporates user specified constraints such as non-negativity, which aid in the stability and interpretability of the factorization. In addition, the choice of data structure for representing a sparse tensor affects performance in ways such as memory bandwidth, number of floating point operations (FLOPs) performed, and opportunities for parallelism. To that end, CPstream uses the compressed sparse fiber (CSF) data structure designed by this research group and illustrated in Figure 2: CSF can be thought of as a generalization of the compressed sparse row data structure for matrices. The CSF data structure represents a tensor as a forest of "I" trees where "I" is the total number of positions or dimension of the first index of the tensor denoted by "i", with each mode recursively compressed, one after the other, and stored in the next level of the tree. Each path from a root to leaf leads to one tensor non-zero entry. An evaluation of CPstream demonstrated that it converges faster than state-of-the-art streaming algorithms, while achieving lower reconstruction error by an order of magnitude. They also evaluated it on real-world sparse datasets and demonstrated its usability in both network traffic analysis and discussion

Results

- Two peer reviewed conference publications and presentations at the Society for Industrial and Applied Mathematics (SIAM) International Conference on Data Mining and at the International Conference On Parallel Processing.

tracking. Their evaluation uses exclusively public datasets and their source code is released to the public as part of SPLATT (Surprisingly ParalleL spArse Tensor Toolkit), an open source high performance tensor factorization toolkit.

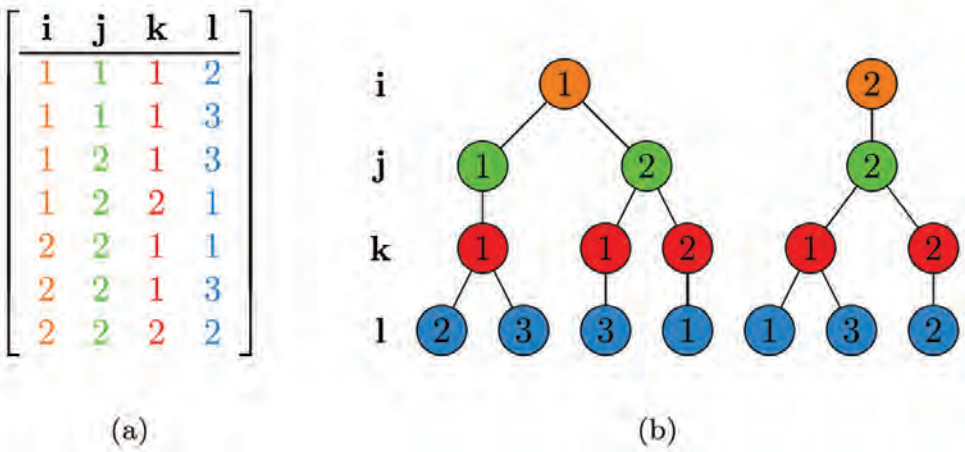


Figure 2: Data structures for the sparsity pattern of a four-mode tensor. (a) Coordinate format: non-zeros are represented as an uncompressed list. (b) CSF format: the sparsity structure is recursively compressed and non-zeros are stored as paths from roots to leaves.

Way Ahead

The research team will continue to enhance SPLATT with a focus towards extending SPLATT's current serial algorithms to high performance parallel formulations and the efficient parallel training of graph convolutional neural networks. This will extend SPLATT's applicability to a greater number of Army systems including Army mission command centers, Army High Performance Computing centers, and Army machine learning applications.

Information Assurance Program

Current Scientific Objectives

01

Create scientific principles of proactive cyber defense using adaptation and deception, and establish metrics for quantifying effectiveness to help build more robust and resilient Army cyber systems.

02

Exploit new security mechanisms, and leverage physical properties and characteristics to develop cutting edge proactive cyber defense techniques for cyber warfighters.

03

Establish Cyber Situational Awareness frameworks that include(s) new cross layer models for dependency analysis, vulnerability and compromise prediction, and cyber triage so that cyber defenders will be able to take more effective actions to mitigate potential intrusions.

Program Manager

Dr. Cliff Wang

Program Manager, Information Assurance Program
Division Chief, Computing Sciences
ARO Information Sciences Directorate

Dr. Wang received his Ph.D. in Computer Engineering at North Carolina State University. He came to ARO in 2003 as the Program Manager for the Information Assurance Program and was promoted to Division Chief, Computing Sciences Division in 2007.

SUCCESS STORY

Automatic Data Triage for Better Cyber Defense

ARO funded research at Penn State University has **created an automatic cyber data triage system that can eliminate repetitive initial data analysis** in order to increase the effectiveness and accuracy of cyber defense.

Challenge

Cyber information consists of a huge amount of heterogonous, data ranging from sensor output to system configuration, coupled with real-time threat intelligence and mission requirements. It is extremely difficult to build an effective data model that pieces them together to generate an overall strategic view for the cyber defense analyst. A lack of concise representation of ground truth while trying to comprehend intelligent adversarial actions, which could be slow and stealthy, poses the biggest and most critical challenge for cyber analysts to establish situation awareness (SA) in the cyber space.

Action

The ARO PM identified the critical importance of establishing cyber situational awareness (CSA). Dr. Wang organized two workshops to explore the topic area and to grow the research community. He successfully initiated a new Multi-disciplinary University Research Initiative (MURI) project on CSA and identified a unique research opportunity at the Penn State University to establish a scientific foundation for cyber security. The Penn State team has carried out extensive research in several key CSA research areas to build situational awareness for better cyber defense. Given the complexity of today's cyber systems, cyber analysts are overwhelmed with a large amounts of data. The current stovepipe type of tools may not be intelligent enough to enable analysts to answer questions such as "what has happened or what should be done?" While many software and hardware tools may help cyber analysts, they typically can't answer these questions as accurately as experienced cyber analysts. Quite often, each tool typically has a narrow focus. Dr. Wang facilitated an information exchange

This success supports these ARL Core Technical Competencies:

Network and Information Sciences

Computational Sciences

This success was made possible by the following ARO S&Es:

- Dr. Cliff Wang, ARO Computing Sciences Division

meeting for Penn state researchers to shares ideas with ARL scientists, and get input from cyber analysts. Using experiences learned from interviewing cyber analysts at ARL, Penn State researchers have focused their research on how to overcome one of the main challenges in cyber data analysis; the substantial amounts of analysis work repeatedly done by human analysts. If an intelligent agent can assist with the repeated work, then the analysts can spend more time dealing with previously unseen cyber-attack situations. A successful research outcome from this team will help create new techniques that fill the gap between "not very intelligent" data processing by tools and experienced analyst's mental processes that build a more comprehensive CSA.

Result

In building CSA, the first time-consuming step cyber analysts perform is data triage, which involves an analyst examining the details of various data sources, such as system configuration data, intrusion system alerts, and firewall logs, in order to weed out false positives, and then link the related indicators together to see the big picture of an ongoing attack. Quite often, the first step to identify attack paths among multiple heterogeneous data sources is a repetitive task for security analysts, even if the same type of attack path was analyzed before. These repetitive tasks are often very time-consuming and severely impact an analyst's ability to perform more critical analysis.

The Penn State research team has developed a technique that could reduce analysts' workloads by automating this process and significantly improving the performance of security analysts. Using a finite state machine, a computational model that can be used to simulate sequential logic, the team successfully constructed a technique to conduct automatic data triage of repetitive tasks that analysts regularly handle. Leveraging principles in both computer science and cognitive science, the new approach combines non-intrusive tracing of human data-triage operations, formal constraint graphs, and data mining of operation traces. The finite state machines are "mined" out of operation traces. In their study, the researchers traced 394 data triage operations of 29 professional security analysts. They utilized the finite state machines to recognize attack-path patterns in more than 23 million firewall log entries, and more than 35,000 intrusion alerts collected from 48-hour monitoring of a network with 5,000 hosts. By comparing the performance of the automated data triage with ground truth, the team found that the automated method generated comparable performance to human analysts, with a low false positive rate. The research findings were published in the March 2019 issue o*f Institute of Electrical and Electronics Engineers (IEEE) Systems Journal.* This advancement will lead to new tools that will potentially free up to 70% of the time that a typical cyber analyst spends each day on repeated tasks, enabling a more efficient warfighter.

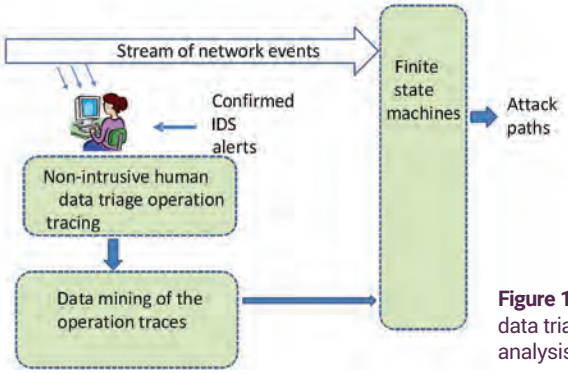


Figure 1: Overview of the proposed cyber data triage method, using finite state machine analysis

Results

- Co-publication between ARL CISD scientists and Professor Liu in *IEEE System Journal*
- Professor Liu gave an invited seminar at ARL CISD and initiated a technology transition proposal
- Penn State team is working with Intelligent Automation Inc. to commercialize CSA research outcomes in mitigating ransomware damage.

Way Ahead

CCDC ARL has been collaborating on this research. Penn State lead principle investigator (PI), Professor Liu, has visited ARL to give an invited talk and explore joint research going forward, which will focus on adopting machine learning techniques to help in depth analysis of cyber-attack data. Initial research outcomes showed very promising results with a high accuracy combined with low false positive rate.

The potential Army impact of this research is the use of this new cyber data triage capability to enhance its cyber operations. Adaptation of this data triage technique into mobile systems defense will also help protect Army tactical communication systems deployed worldwide.

SUCCESS STORY

Establishing Models and Metrics for Cybersecurity Dynamics

ARO funded researchers at the University of Texas - San Antonio **created the first metrics framework for measuring cyberattack and defense agility** that in the long term could provide new applications in cyber security.

Challenge

Although there are many cyber security defense mechanisms and approaches, the significant challenges in cybersecurity is that it is unknown how to form a holistic perspective and quantify effectiveness of cyber actions. This is exacerbated by a lack of well-defined cyber security metrics. Quite often we cannot address questions such as: How do we measure the success in terms of defeating an ongoing attack? How can we quantify the pace at which cyber attackers are outmaneuvering, or being outmaneuvered by, cyber defenders? This problem is important because dynamic strategies and quick actions are commonly used by both cyber attackers and defenders. For example, cyber attackers often adapt their strategies when new software vulnerabilities are discovered and/or mitigated, and cyber defenders often adapt their strategies when new attacks are detected. This leads to the scientific challenge of quantifying cyber-attack and defense agility and maneuvering actions.

Action

The ARO PM first identified the critical importance of establishing models and metrics for cyber security operations. For the past several years, he has teamed with ARL scientists to tackle the challenge. After identifying Dr. Shouhuai Xu's, of the University of Texas - San Antonio (UTSA), interests in working on this problem, Dr. Wang established a formal model and metrics for cyber security with Dr. Xu. Dr. Wang also funded Professor Xu's research through the ARO single investigator program. Through information exchange meetings, Dr. Wang introduced Professor Xu's work to collaborating ARL scientists. To extend the initially funded work by ARO, ARL provided additional funding to support Professor Xu's.

This success supports these ARL Core Technical Competencies:

Network and Information Sciences

Computational Sciences

This success was made possible by the following ARO S&Es:

- Dr. Cliff Wang, ARO Computing Sciences Division

Results

- Professor Xu and his ARL collaborator proposed the first metrics framework for measuring cyberattack and defense agility that could help cyber defenders
- Research results were published in *IEEE Transactions on Information Forensics* and *Security*
- Professor Xu's research won the 2019 world-wide Adversarial Malware Classification Challenge organized by the MIT Lincoln Lab

Results

In cyberspace, dynamic strategies are quite often used by both attackers and defenders, hoping to gain an advantage over the opponent. However, in order to win, it is important for the cyber defender to have a set of quantitative metrics that would characterize the effectiveness of both attackers' and defenders' cyber agility maneuvers. Despite its clear importance, few systematic metrics have been developed to quantify the cyber agility of both attackers and defenders. In order to tackle this problem, Professor Xu and his collaborators created an innovative approach, dubbed "synergistic concept-driven and data-driven analytics," with the basic idea to seek first-principle new concepts that can describe and represent cyber attack and defense agility, and use data to validate these new concepts. They proposed the first metric framework for measuring cyber agility in terms of the effectiveness of their dynamic moves by both cyber attacks and defenses. The metrics mainly focuses on measuring the timeliness and effectiveness to capture the core concepts of agility. The proposed framework is generic and will transform any relevant, quantitative, and/or conventional static security metrics (e.g., false positives and false negatives) into metrics capturing system dynamic behaviors. The team has carried out case studies using two real-world datasets. The results show that the proposed metrics provide valuable insights for a defense strategy because they allow a defender to measure several aspects of cyber agility. These aspects include the defender's own responsiveness to attacks over time, the identification of which defense changes have been targeted by attackers, and the ongoing effectiveness of the defender against a single or set of attackers. Insights derived from these metrics will enable the defender to become more responsive, more targeted, and more effective in their competition to out maneuver attackers.

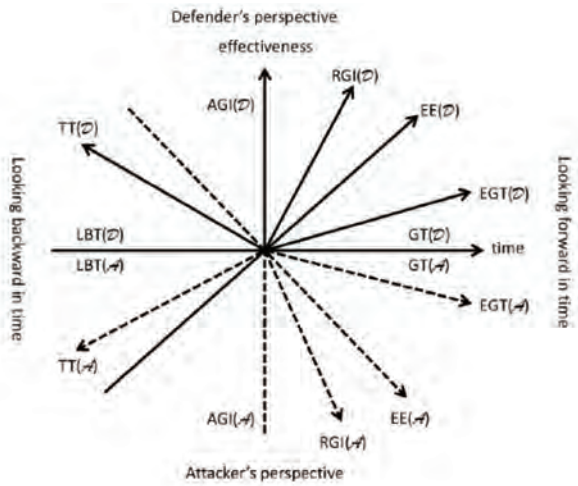


Figure 2: The structural relationship between the 14 cyber-attack and defense agility metrics, structured around two dimensions: *time* and *effectiveness*. Intuitively, the metrics geared towards time (the x-axis) look both forward and backward in time, while the metrics geared towards effectiveness (the y-axis) look at both the attacker's and defender's perspectives.

Way Ahead

CCDC ARL scientists have been collaborating on this research. Professor Xu will continue his work to define metrics and model for quantifying cyber defense actions and build a holistic model that can capture the dynamic actions between attackers and defenders through multiple stages of engagement.

The potential Army impact of this research is that the model and metrics will help Army cyber defenders plan and carry out effective cyber defense actions, and assess their mission success level. A holistic view provided by the cyber dynamics model will also help cyber defenders to gain an improved situation prediction capability through multiple, concurrent scenario analysis.

Information Processing and Fusion Program

Current Scientific Objectives

01

To achieve a deep understanding of data in all its structured and unstructured forms, and to discover comprehensive but simple models and algorithms, that if successful will advance the state-of-the-art for perception and control to enable refined decision making for robotic agents, and will help improve military and civilian security, and safety through smart persistent sensing.

02

To intelligently harvest quantitatively meaningful information from today's ubiquitous and diverse sensing of environments for a subsequent creative weaving/fusion into full scene understanding that if successful, will enable rapid situational awareness, alleviate surprise, and provide tools for a suitable response to imminent and unforeseen danger, bringing closer the reality of "anytime, anywhere" sensing autonomy for the future Army.

Program Manager

Dr. Hamid Krim

Program Manager, Information Processing and Fusion

Computing Sciences Division

ARO Information Sciences Directorate

Dr. Krim completed his B.S. in Electrical and Computer Engineering and M.S. in Applied Mathematics at the University of Washington, and his Ph.D. degree at Northeastern University. He joined ARO in 2019 as the Program Manager of the Information Processing and Fusion Program.

SUCCESS STORY

Brain Computer Interface: First Cross-Monkey Message Decoding

A new capability of **detecting and interpreting brain signals** holds the promise of uncovering a Soldier's state of readiness and attention.

Challenge

Sensing, understanding, and exploiting human sensorial information is important in a number of Army applications. A significant objective of neural engineering is to design robust and reliable brain-computer interfaces (BCI) that generalize well over a large

This success supports these ARL Core Technical Competencies:

Human Sciences

Computational Sciences

This success was made possible by the following ARO S&Es:

- Dr. Hamid Krim, ARO Computing Sciences Division

population of subjects. Such cross-subject BCIs should be trained over a limited number of representative subjects, and are expected to perform reliably over unseen representatives from the same population. Central to such BCIs is the cross-subject decoding problem, in which training data collected from one representative subject, is used to train a reliable decoder for another subject. This is a challenging neurological problem. The great difficulty lies in the high variability of neural signals in light of the dramatic variation of their statistical properties, under a slight change in the recording conditions. In other words, the feature spaces where the actual decoding of actions is performed varies across the population.

Action

The ARO PM has discussed with scientists from the CCDC Soldier Center, who noted the existing gap in BCI research despite its crucial potential to serve many Soldier-centric needs as well as its broader impacts on DoD and Army human-systems interactions. A Multi-disciplinary University Research Initiative (MURI) topic was put forward, "Closed-Loop Multisensory Brain-Computer Interface for Enhanced Decision Accuracy," and was eventually awarded to Dr. Maryam Shanechi from the University of Southern California as the Lead Principal Investigator.

While brain signals have long been of interest in many contexts, accounting for multi-sensory cues of a human brain engaged in some activity under duress or pressure, and feeding back the information with a goal of possibly sharpening the decision making, i.e. closing the loop, is new. Typically, other physiological measurements have been taken, e.g., blood pressure.

Result

Professor Tarokh, from Duke University, along with co-investigator Professor Pesaran, from New York University, and other graduate students have been able to realize the brain decoding of eye saccade movements of one monkey by another monkey. This is the first such experiment achieved in the laboratory. With their newly developed "centering" algorithm, they were able to decode brain signals sensed at implanted probes in a monkey's brain, and apply them to probes implanted in another monkey's brain, and get the latter to repeat the action of the former.

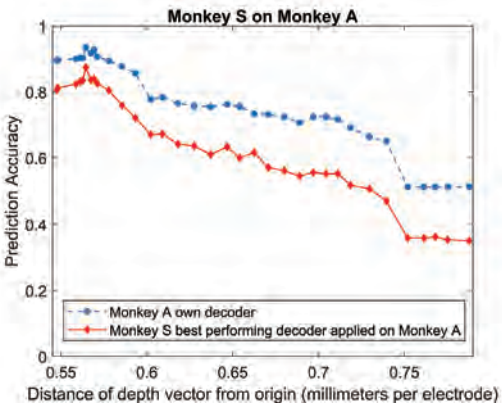


Figure 1: Performance of cross-monkey decoding.

Way Ahead

The Army impact of this research is its possible adoption in reducing the multi-tasking challenge faced by Soldiers, for example helicopter pilots, in an unknown and/or hostile environment. Other broader impacts may include inspiring future artificial intelligence and machine learning (AI/ML) algorithm design, and the choice of informative features to secure superior and robust performance of all Army Soldiers, in the presence of uncertainty and unexpected battlefield conditions. The ARO PM will introduce the research results to key CCDC ARL in house researchers and establish collaborative research going forward.

Results

- Three conference papers have been published and one journal paper in a neuro-science and machine learning journal is under way
- This research could facilitate the detection of a Soldier's state of mind to enable preventative actions and alerts for the Soldier (e.g. fatigue detection that alerts the Soldier)
- These results are moving towards building a read and write capacity of brain patterns to help increase a Soldier's resilience in a battlefield (e.g. helicopter pilot mental fatigue)

SUCCESS STORY

Real-time Multimodal Event Detection

The newly developed strategy would yield a **total prediction of the collective behavior of a crowd following a short observation of some of the group's characteristic signatures**. This could enable better situational awareness in crowded areas of operation.

Challenge

In numerous and important Army tasks, event detection is central and also crucial to many surveillance applications of military and civilian nature, including border security, sensitive facilities oversight as well as cyber-security. The associated challenge lies in the varying nature of the threat and its manifestation which in turn, requires a diverse body of sensors which are often incompatible. To palliate such a challenge and help obtain actionable information, a variety of sensors such as cameras for imagery, video, and auxiliary information such as signals intelligence (SIGINT), may typically be deployed. Of keen interest in Army battlefield operations as well as other civilian homeland security applications, is acquiring such information in real time to enable a quick adaptation to the evolving information on the ground. The fusion of this data, utilizing effective and efficient techniques, to create actionable intelligence for real-time event detection is critical to the success of military and law enforcement missions.

Action

Information non-commutativity is rather pervasive and has been observed in many important applications. For example, in distributed sensor networks or social networks, information flow strongly depends on network topology, by following the shortest path or any other protocol. Information non-commutativity has in fact been investigated in quantum information sciences.

This hindsight, together with the long experience of the PM in the area of sensor fusion, and the potential cost or design benefit of combining sensors, led to the question of general practicality of such option. The importance of this information and its causal properties are clearly crucial to AI applications and surveillance, which are of critical importance to Army Modernization priorities, such as autonomy or command, control, communications, and intelligence. Discussions with Army laboratories and other DoD researchers and PMs, led the PM to further develop the idea and propose a MURI topic on "Adaptive Exploitation of Non-Commutative Multimodal Information Structure." This MURI was eventually awarded to a team led by a Principal Investigator from University of Illinois at Urbana-Champaign. Primarily driven by causality of information, the research activity is proceeding with a guidance of Army Modernization priorities in mind.

Result

Professor Tarokh (from Duke Univ.) and his graduate students along with ARL researchers (Dr. L. Kaplan) have developed a real time working fusion algorithm (maybe the first) and the associated theoretical framework to detect anomalies which can also be viewed as potential threat detections. The newly developed theory is based on

This success supports these ARL Core Technical Competencies:

Network and Information Sciences

Computational Sciences

This success was made possible by the following ARO PM:

- Dr. Hamid Krim, ARO Computing Sciences Division

Results

- Published two journal papers in the Institute of Electrical and Electronics Engineers Transactions on Information Theory and seven conference papers
- Methodology and associated software were presented to ARL for potential future studies to adapt for management of mob-like riots or insurgent activity in urban settings
- Potential development of a real time response, hand-held tool that could be fielded to Soldiers for better tactical situational awareness

Partially Observed Markov Decision Processes, and directly uses multi-modal data to monitor an event (e.g. public gathering) to flag a change in the level of non-stationarity of the statistics of data of interest to ultimately provide structural results for the optimal decision policy.

In demonstrating the applicability of this technique to military and civilian security assurance problems, this technique was used to investigate data collected around an event in New York City (NYC) with multi-modal data consisting of closed circuit television (CCTV) imagery and social media posts to detect a 5K run in New York City. Physical sensor data from CCTV cameras and social media data, from Twitter and Instagram were the multimodal information collected before/after/during the Tunnel2Towers 5K run/walk that occurred on Sunday, September 25th, 2017.

The system as shown in Figure 2a exploited Tweets and Instagram posts near the CCTV cameras by processing videos to coherently combine the information converted to counts and into a decision. Figure 2b shows the timely detection of the event and its time stamp, including the whole time preceding the event.

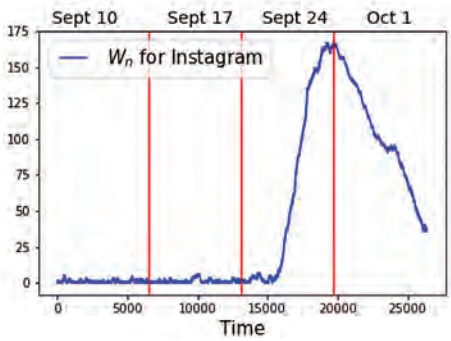


Figure 2:A: Algorithmic realization of the event detector.

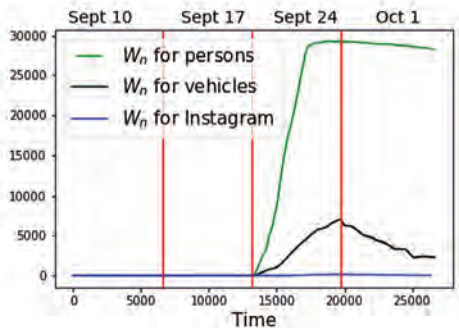


Figure 2:B: Test statistics marking the onset of event.

Way Ahead

The Army impact of this research includes surveillance for quick situational understanding and awareness in a mission-specific task around an area, as well as other security-driven monitoring, environmental search-and-rescue applications and a number of other civilian applications. The ARO PM with the help of ARL researchers familiar with the research findings, will introduce the results to other key CCDC ARL in house researchers and Army Corps going forward.

Intelligent Systems Program

Current Scientific Objectives

01

Create new methodology and techniques in machine learning emphasizing online learning methods that if successful, will increase the flexibility and resilience of unmanned systems enabling Soldiers to deploy these systems in complex and poorly understood environments

02

Enable efficient and effective knowledge representation, reasoning, and decision making in long duration missions in open worlds that if successful, will support future Army requirements for unit self-sufficiency during extended missions

03

Devise new methods that enable autonomous systems to interact with other entities in physical and cyber spaces that if successful, will enable intuitive communication between Soldiers and autonomous systems such as robots, swarms or decision aids

04

Create rigorous theoretical underpinnings and tools, such as testing methodologies and self-evaluation, to enable assured operations and ensure the safety and reliability of the Army's future unmanned systems

Program Manager

Dr. MaryAnne Fields

Program Manager, Intelligent Systems Program

Computing Sciences Division

ARO Information Sciences Directorate

Dr. Fields received her B.S. degree in Mathematics at the University of Louisville, her M.S. degree in Mathematics, and her Ph.D. in Mathematics at Clemson University. She began working for the Army as a mathematician in 1989. She came to ARO in 2019 as the Program Manager for Intelligent Systems.

SUCCESS STORY

Systematically Studying Backdoor Attacks on Deep Neural Networks

ARO funded research developed **methods to predict and identify cyber-attacks that can target sensor systems**, that in the long term will improve the safety and reliability of future intelligent systems used by the Army, such as sensors for targeting and reconnaissance.

This success supports these ARL Core Technical Competencies:

Network and Information Sciences

Computational Sciences

This success was made possible by the following ARO S&Es:

- Dr. MaryAnne Fields, ARO Computing Sciences Division
- Dr. Cliff Wang, ARO Computing Sciences Division

Results

- Dr. Li's team presented a peer reviewed conference paper "Defending Neural Backdoors via Generative Distribution Modeling" at Thirty-third Conference on Neural Information Processing Systems
- Researchers won first place in defense at the CSAW'19 HackML competition at New York University techniques developed in this project, where the method detected both maliciously added backdoors and naturally occurring back doors

Action

Based on the challenges outlined above and the Army's interest in autonomous technologies for both its Next Generation Combat Vehicle and Future Vertical Lift platform, the previous Intelligent Systems PM, Cliff Wang, recruited Dr. Hai Li of Duke University to conduct a seedling project to systematically study backdoor attacks on DNNs. Such research could have a significant impact on applications, such as perception systems, that depend on deep neural networks and very large datasets. Developing techniques to recognize and mitigate backdoor attacks will improve the safety and reliability of future intelligent systems.

Results

Current approaches to defending against backdoor attacks in computer vision attempt to recover a single estimate of a trigger by minimizing the loss between triggered images and known examples of a given class. However, typical generative models such as, generative adversarial networks and variational autoencoders, require samples of both legitimate and "hacked" examples which are unavailable for back-door attacks. Dr. Li's group uses a sample-free approach to generate a distribution of triggers that can successfully deceive the DNN. This probability distribution cannot be directly sampled, but it can be related to the observable Attack Success Rate (ASR) function. Dr. Li and her team used a maximum entropy staircase approximator (MESA) approach to learn the trigger distribution from a group of sub-models, each of which learns a portion of the trigger distribution. Figure 1 illustrates the MESA algorithm.

Experimental results show that MESA can effectively recover the valid trigger distribution on various types of triggers, and significantly improve the defense robustness. Dr. Li exhaustively tested 51 representative 3x3 binary triggers on the Cifar10 dataset, and also random color triggers on Cifar10/100 dataset. She was able to show that using the 3x3 binary trigger distribution to retrain the original DNN, reduces the ASR from greater than 90% to less 10%. In the CSAW'19 HackML competition, students from Dr. Li's group won first place in backdoor defense, using the techniques developed in this project to recognize and defend against back door attacks in a facial recognition task. In this setting, they were able to defend against both malicious and natural triggers. Natural triggers occur when hats, glasses, or other objects become associated with specific individual in the database.

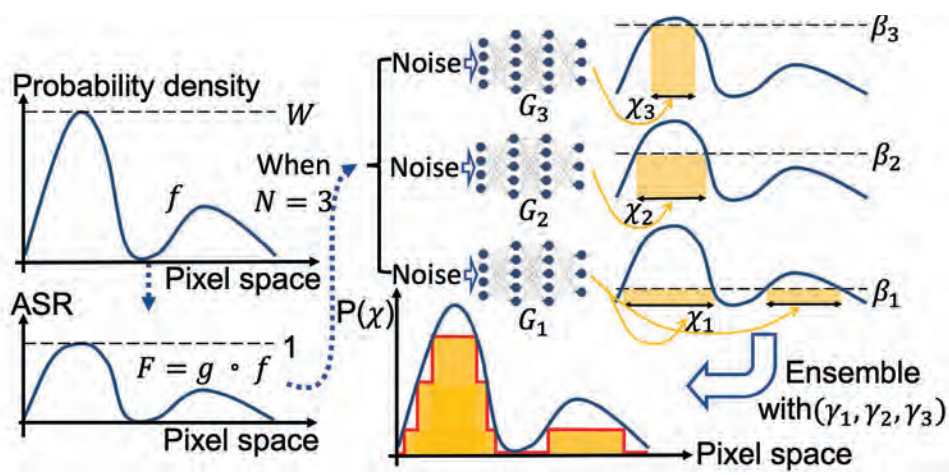


Figure 1: The principal idea of the MESA is to approximate the probability density function, f, by an ensemble of N sub-models G1,G2; ...,GN, and let each sub-model Gi only to learn a portion of f. The partitioning of the ASR function follows the method of staircase approximation and truncates the range [0,1] into N levels defining the support sets Xι (in pixel space) as illustrated by the yellow rectangles in Figure 1(a). The sub-models Gi; learn the corresponding sets Xι associated with each level. Both F (ASR) and f (the pdf) can be reconstructed as a combination of the sub-models.

Way Ahead

The current implementation of Dr. Li's work only considers non-structured backdoor triggers with fixed shapes and sizes. It is also assumed that the trigger size is known by the defender. In the future, these limitations can be addressed within the current MESA framework extending the techniques to trigger distributions of all shapes within the maximum size of the generator's output. These techniques will improve the safety and robustness of the Army's future autonomous vehicles and other perception systems.

Biomathematics Program

Current Scientific Objectives

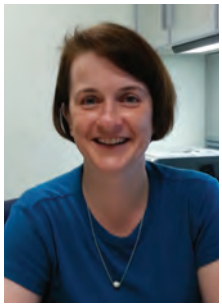
01

Develop the mathematics and models for understanding circadian dysrhythmia-related illnesses, in particular those relating to sleep, that, if successful, is anticipated to lead to improved Soldier health and performance

02

Develop the mathematics and models for discovering and characterizing the complex host-microbe and microbe-microbe interactions occurring in skin microbial communities to enable microbial community manipulation to modify body odors, maintain health, and enable novel microbiota-mediated capabilities to protect the Soldier

Program Manager



Dr. Virginia Pasour

Program Manager, Biomathematics

Mathematical Sciences Division

ARO Information Sciences Directorate

Dr. Pasour completed her M.S. in Biostatistics at UNC-Chapel Hill in 1995. She trained as an Applied Mathematician at Cornell University, receiving her Ph.D. in Applied Mathematics in 2007. She came to ARO in 2009 as the first Program Manager for the Biomathematics Program.

Information Sciences Directorate

- Computing Sciences Division
- **Mathematical Sciences Division**
- Network Sciences Division
- Technology Integration & Outreach Division
- ARO Special Programs

SUCCESS STORY

Technologies to Target Sleep Disruption in Post-Traumatic Stress Disorder

This ARO initiative resulted in **new connected models of the brain and neuroendocrine system as well as a circadian rhythm monitoring and regulation system**, which will help reduce Post-Traumatic Stress Disorder symptoms through improved sleep.

This success supports these ARL Core Technical Competencies:

Human Sciences

Protection Sciences

This success was made possible by the following ARO S&Es or Program Specialists:

- Dr. Virginia Pasour, ARO Mathematical Sciences Division
- Dr. Frederick Gregory, ARO Life Sciences Division

Results

- STTR-funded PTSD SleepAid game recognized in 2019 by the world's largest modeling, simulation and training event for its innovation and potential to help treat PTSD
- PTSD SleepAid app currently being validated at the University of Central Florida on veterans with PTSD
- The PTSD SleepAid project together with the earlier Circadian Monitoring and Regulation system has resulted in a commercial product, Delux, that has received support from the military psychology community
- Computational Psychiatry workshop planned by PIs, ARO, MRDC, and the National Institutes of Health

Challenge

Understanding post-traumatic stress disorder (PTSD) is not a simple task as there is no reliable biological predictor or marker for PTSD, and diagnoses are heavily reliant on self-reporting. Current treatments include psychotherapy and pharmacotherapy; it is not clear how the two interventions inform each other and they are not always successful. In part, these challenges are due to a lack of comprehensive understanding of the biological processes and systems that are affected by PTSD, and how they respond and interact with each other under stress. In particular, people suffering from PTSD often experience the same emotionally charged dream over and over again. Rapid eye movement (REM) sleep is thought to be important for the consolidation of emotional memories and in particular, it is thought that REM sleep consolidates the content of emotional memories while at the same time reducing their emotional charge. The mechanisms by which this happens are largely unknown.

Action

After deciding on Fundamental Laws of Biology as a high-risk, high-reward area that would be appropriate as a central thrust for the new Biomathematics Program, Dr. Pasour quickly discovered the DARPA FunBio program and steered the first follow-on program, Biochronicity, toward research aimed at gaining a clear understanding of the role and effects of time, in and on human physiology and biological functions.
Dr. Pasour initiated discussions with Dr. Maria D'Orsogna, at California State University-Northridge, and Dr. Tom Chou, at the University of California at Los Angeles, about disruptions of the circadian clock, specifically stress and its relationship to PTSD.
Dr. Pasour collaborated with Dr. Fred Gregory, ARO Program Manager, Neurophysiology and Cognition, the benefit of this research to his program, which culminated in a single investigator proposal that develops dynamical models for the neuroendocrine system.
In 2018, a new grant was awarded for the mathematical modeling of limbic system dynamics, pathophysiology, and response to stress. These grants, in addition to being co-funded by the ARO Biomathematics and ARO Neurophysiology and Cognition programs, were also co-funded by the ARO Historically Black Colleges and Universities/Minority-serving Institutions (HBCUs/MSIs) program. In addition, building upon a previous ARO funded rule-based decision project, principal investigator (PI) Nancy Kopell and Dr. Sujith Vijayan at Virginia Tech met with Dr. Pasour and discussed ideas for a study that models the neural dynamics of emotional memory consolidation, that was funded in 2017.

At a higher level, after authoring a successful circadian-rhythm related Small Business Technology Transfer (STTR) topic on circadian rhythm monitoring and regulation, Dr. Pasour co-authored another STTR topic with Medical Research and Development Command (MRDC) in 2016, which complements the capabilities of the original circadian rhythm regulation device in combating PTSD, specifically by discouraging daytime napping.

Result

The goal of Dr. D'Orsogna's and Dr. Chou's work was developing and analyzing a mathematical model that incorporates the relevant physiological features involved in stress response regulation, including the hypothalamus-pituitary-adrenal (HPA) axis (Figure 1), that receives input from stress and regulates cortisol production in the body. Cortisol is one of the main hormones in the body and aids in regulating

metabolism and mood, among other functions. It is also observed that often, PTSD patients suffer from hypocortisolism, low cortisol production, leading to cortisol levels being used as a possible biomarker for PTSD. Over the course of the first grant, Dr. D'Orsogna and Dr. Chou formulated a more complete and realistic model for the HPA axis, including hitherto neglected processes. Specifically, they distinguished the slow process of cortisol-mediated corticotropin-releasing hormone (CRH) biosynthesis from the fast process of CRH secretion, and were able to reproduce known oscillatory behavior patterns while uncovering the existence of two basins of attraction. One marked by "normal" cortisol levels, the other by hypocortisolism, the "disease" state that is observed in PTSD patients. They found that external distress, such as traumatic events, can lead to transitions from normal to diseased state. This is important because it means that the emergence of hypocortisolism in PTSD patients can be due solely to psychological trauma, and not necessarily because of physical injuries; the latter possibility would change the physiological parameters of the model. They also found that by carefully tuning external stress, the reverse transition from diseased to normal state could be triggered, implying that exposure therapy (i.e. subjecting patients to stressful events in a clinical setting), may help eliminate PTSD symptoms, so that no physical intervention may be necessary. More recently circadian rhythm has been incorporated into the original model, with the finding that the relative phase of the circadian rhythm relative to the onset of external stress can have profound consequences on the resulting dynamics; specifically, the same intensity and duration of external stress can lead to a transition from the normal to the diseased state depending on the time of its onset compared to the circadian rhythm.

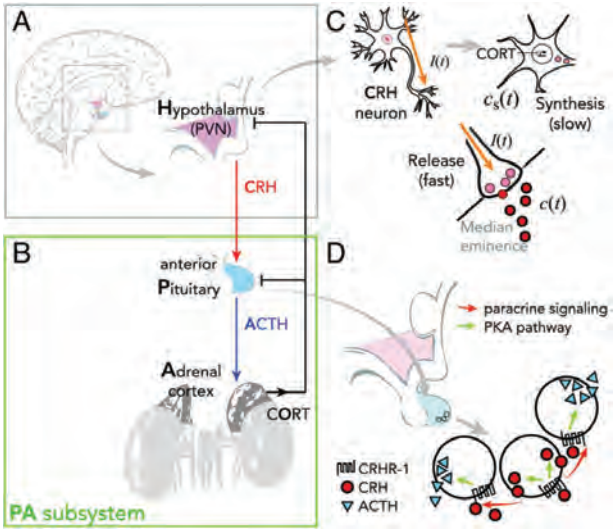


Figure 1: Schematic of the HPA axis. **A.** Stress is processed in the central nervous system (CNS) and a signal is relayed to the paraventricular (PVN) in the hypothalamus to activate CRH secretion into the hypophyseal portal system. **B.** CRH diffuses to the pituitary gland and activates ACTH secretion. ACTH travels down to the adrenal cortex to activate cortisol (CORT) release. Cortisol inhibits both CRH and ACTH secretion to down-regulate its own production, forming a closed loop. **C.** Negative feedback of cortisol suppresses CRH synthesis in the PVN, ultimate reducing the amount of stored CRH and its subsequent release. External inputs such as stressors and circadian inputs directly affect the release rate of the CRH at the axonal terminal. At the axonal terminal, released CRH upregulates its own secretion. This self-upregulation action is mediated by the CRH receptor 1 (CRHR-1). **D.** The protein kinase A (PKA) pathway is a chain of events that involves PKA mediating the corticotropin-releasing hormone (CRH) to adrenocorticotropic hormone (ACTH) production.

Using the new model to examine learning in the amygdala under conditions mimicking REM sleep in PTSD patients, Dr. Vijayan found that plastic changes under PTSD were diametrically opposite to those produced under normal REM sleep conditions – these differential effects of neuromodulator conditions on plasticity may be the key to the pathophysiology observed in PTSD patients. The amygdala engages both fear expression and fear suppression pathways, but the connectivity and the proportion of amygdala cell types that engage these two pathways differ. One possibility is that under REM conditions, the fear expression pathway is weakened and/or the fear suppression pathway is strengthened, thus reducing the emotional charge of a memory while strengthening the content, a phenomenon seen in experimental work. In contrast, the conditions of PTSD may result in the strengthening of the fear expression pathway and/or the weakening of the fear suppression pathway, thus resulting in the same emotional dream being experienced over and over again by PTSD patients.

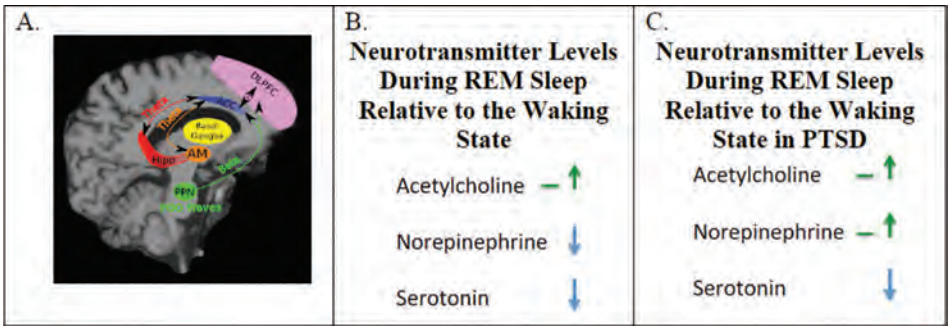


Figure 2: A. Proposed circuit for emotional memory consolidation. Rhythmic interactions between the anterior cingulate cortex and the dorsolateral prefrontal coretx (via the theta and beta bands) along with rhythmic input from the limbic structures (via the theta band) help to consolidate emotional memories. PGO waves trigger the selection and evaluation of emotional memories by the DLPFC and the ACC. The amygdala provides the emotional content while the hippocampus provides contextual information via the theta band. B. Activity during REM sleep occurs under different physiological conditions. Acetylcholine levels are similar to waking conditions while norepinephrine and serotonin are much lower. These changes in neurotransmitter levels may be key to consolidating the content of emotional memories while reducing the charge of the emotional valence. C. In PTSD patients norepinephrine levels remain high during REM sleep. This aberration in norepinephrine levels may prevent the emotional valence of memories from being reduced, resulting in the reliving of an emotionally charged dream night after night. PPN = Pedunculopontine tegmental nucleus, AM = amygdala, and Hipp = Hippocampus.

Service members with PTSD have demonstrated a tendency to take daytime naps, that results in the inability to obtain a deep sleep at night. Hyperarousal, a state of high physical alertness common with PTSD, must be reduced to improved sleep. The STTR topic co-authored with MRDC uses wearable sensors with a mobile app in order to provide correction of circadian rhythm disruption, recommendation for physical and mindfulness exercises using innovative sleep-wake, and activity and arousal detection models, and uses goal-oriented, game-based intervention to enhance user engagement to prevent daytime napping.

Way Ahead

In August, 2018, Dr. Marti Jett, MRDC, attended the Technical Assessment Board review of the Mathematical Sciences Division of ARO's Information Sciences Directorate. She performs experimental work related to PTSD and was particularly interested in Dr. Pasour's presentation of Dr. D'Orsogna's and Dr. Chou's work. Dr. Pasour organized a discussion between Dr. Jett, Dr. D'Orsogna, and herself, which resulted in leveraging Dr. D'Orsogna's current position as Associate Director of the Institute for Pure and Applied Mathematics (IPAM) at UCLA in order to bring the PIs doing circadian-rhythm-related work, and other leaders in the field for a technical information exchange and stimulate collaborations. The exchange will specifically explore how modern computational tools and mathematical modeling can be integrated with measurements to improve psychiatric diagnosis and treatment. Along with Dr. Jett from MRDC, Dr. Pasour, and several academics, Dr. Shashaank Vattikuti, NIH, is also a member of the organizing committee. The workshop will be held February 18-21, 2020.

In addition, auditory stimulation during sleep has already shown promise as a tool for influencing sleep architecture and functionality in experimental studies. For example, studies have shown that the covert introduction of task-related auditory cues (e.g., sounds present during learning) during sleep enhances sleep-related learning and memory benefits. Surprisingly, even non-task related auditory cues, when appropriately timed

during sleep oscillations, can increase the amplitude of slow-wave sleep oscillation, enhance sleep-related learning and even engaged the immune functions of sleep. However, the optimal sequence, timing, and form of the auditory stimulus have yet to be investigated. In 2019 Dr. Pasour discussed the possibility of using the biophysically based computational models from Dr. Vijayan's current grant to identify candidate acoustic stimulation protocols for either the enhancement of memory, or the prolongation of sleep; the candidate stimulation protocols could then be tested experimentally. As a result of this discussion, Dr. Vijayan has submitted a white paper and proposal to the ARO Biomathematics Program that would employ the REM sleep models developed for this project as part of plan to study auditory stimulation, and the ability to enhance learning or treat disorders in which abnormal sleep dynamics are present.

The proposed auditory stimulation device has the potential to optimize the considerable power of sleep to prime a Soldier for action, and may also be tailored to different circumstances. If successful, the results could also be used to prolong sleep and reinstate normal sleep architecture in traumatic brain injury (TBI) patients and restore normal brain rhythms during REM sleep in PTSD patients, thus alleviating the symptoms in both disorders.

The PTSD SleepAid game was a finalist at the Serious Game Showcase & Challenge and is available in the Google Play Store. In addition, a combination of the PTSD SleepAid project and the Circadian Monitoring and Regulation (CMR) system has resulted in a commercial product, Delux, that has received support from a Command Psychologist at Joint Base Langley-Eustis.

SUCCESS STORY

Understanding the Skin Microbiome

This ARO initiative resulted in the **discovery and characterization of the complex host-microbe and microbe-microbe interactions occurring in the skin microbiome** in order to recognize and produce skin microbial communities exhibiting optimal properties, such as reduced attraction of insects, and reduced disease occurrence.

Challenge

The effectiveness of our first line of defense against infection, the skin, is controlled in part by a dynamic microbiome, yet the mechanisms of these interactions are not well understood. For example, most humans have skin microbial communities that exclude specific pathogens, such as the virulent soft tissue pathogen *Staphylococcus (S.) aureus*, but researchers have found that *S. epidermidis*, which forms part of the human skin microbiome, can exclude *S. aureus*. Skin microbes also cause other effects such as producing volatile compounds that attract biting insects, cause body odor, and likely act as subliminal social cues. Until recently, it was impossible to collect the data necessary to conduct fundamental studies on these intricate skin-microbe and microbe-microbe interactions; breakthroughs in DNA sequencing and technical achievements in metagenomic library construction now enable never before possible, collection of the requisite data.

This success supports these ARL Core Technical Competencies:

Human Sciences

Protection Sciences

This success was made possible by the following ARO S&Es:

- Dr. Virginia Pasour, ARO Mathematical Sciences Division
- Dr. Robert Kokoska, ARO Life Sciences Division

Action

In the year 2010, a Multi-disciplinary University Research Topic (MURI) topic on the skin microbiome was developed to investigate the possibilities of leveraging the technological and informational advances generated by the sizable NIH Human Microbiome project, that was directed at characterizing and relating primarily non-skin microbiota to disease states. The ARO Microbiology Program was particularly interested in the possibility of manipulating the skin microbiome to discourage the biting of disease-carrying insects, such as malaria-carrying mosquitoes, while Dr. Pasour was interested in applying mathematical modeling methods typically used in studying traditional ecosystems to developing our knowledge of this nonstandard but important ecosystem. The topic went forward and was awarded in 2012 to Johns Hopkins University/Applied Physics Lab with Dr. Dave Karig as the PI. Dr. Bob Kokoska, ARO Program Manager, Microbiology, took over as the co-monitor role in 2013.

Result

The purpose of this work is to explain skin health and disease in terms of maintenance and disruption of the ecology of complex microbiomes. This requires identifying factors governing community specificity across sites and individuals, and community assembly dynamics that result from changes in the environment, host state, or exposure to microorganisms. Toward these goals, Dr. Karig and his team implemented protocols for spatially resolved sampling of forearm and forehead environments, which range in moisture content, sebum content, pH and temperature, and have been demonstrated to host taxonomically diverse microorganisms. A major challenge was quantifying data from low abundance sites, and over the course of the project, the team developed improved sequencing techniques and bioinformatics classification for characterizing the microbial communities associated with skin samples. In addition, they explored, both theoretically and in vitro, a range of mechanisms known to influence microbial community structure (e.g., resource utilization, competition, dispersal and spread, microbial division of labor). Finally, they have considered broad scale patterns in bacterial distributions, abundances, and co-occurrences that can be used to formulate hypotheses on underlying mechanisms of community assembly (e.g., colonization resistance).

Ecological modeling, including both statistical analysis and dynamical systems, was used to synthesize detailed observations of microbial distribution patterns, and their potential mechanistic causes. Both intra-site, and interpersonal variation have been studied, with random forest analysis implying the existence of a core microbiome within sites, indicating that ethnicity and certain lifestyle factors (e.g. diet) are strong drivers of microbiome composition. Moreover, the modelers performed a trait-based analysis of the human skin microbiome and developed Granger causality techniques for microbiome data. They also published a simulation model to examine when contamination is likely to be problematic, relating the degree to which sequencing results are influenced by contamination to sample characteristics such as DNA input, as well as ecological characteristics such as taxon diversity. Through add-on funding, a mathematical model was created for inflammation and proliferation stages of wound healing under the threat of P. aeruginosa infection within the dermis. The model considered white blood cells, P. aeruginosa, and fibroblasts as individual stochastic agents who interact through the uptake and release of chemoattractants and nutrients, modeled by partial differential equations. In addition, mechanistic modeling has

Results

- Invited presentations at the DoD Tri-Services Microbiome Consortium (TSMC) Special Topics Meeting (June 4, 2019, Framingham, MA), at the Synthetic Biology for Defense Workshop (SB4) in Arlington, VA (September 25-27, 2018), and at the TSMC Symposium (October 22-24, 2019)
- Collaboration with scientists at Fort Benning on analysis of microbiomes for recruits
- Collection of over 900 microbial isolates to be made available to the scientific community
- Software to facilitate experimental microbiome work (KrakenUniq, Centrifuge, and Pavian) available via GitHub

been integrated with machine learning to predict the conditions of persistence for a mutualistic system.

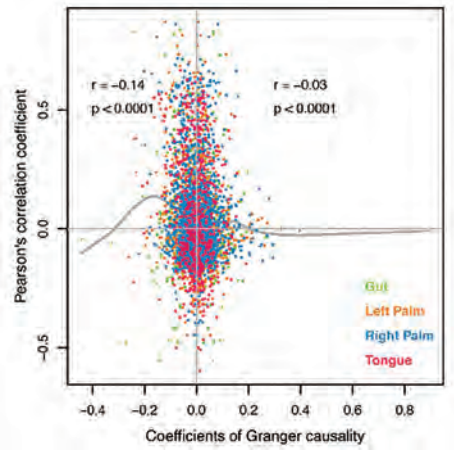


Figure 3: Granger causality vs Pearson's correlation coefficient for all four body sites. Granger causality (GC) is expressed as change in abundance of response variable (in standard deviation) as the abundance of Granger-cause increases by 1 SD. Positive coefficients indicate positive effect of the Granger-cause on response in affecting abundance, and vice versa. For a given taxon-pair, the highest coefficient among all positive coefficients and the lowest one among all negative coefficients are shown in the figure. The relationship between Pearson's correlation and Granger causality is shown separately for positive GC and negative GC along with separate splines.

Way Ahead

As a part of the MURI research, a number of products of different types have resulted. In the realm of experimental resources, a collection of over 900 microbial isolates was made, and the MURI team is working with BEI Resources in order to share a representative set with the community. In addition, microfluidic devices have been developed to facilitate in vitro experiments. Several software tools were developed as well and are available via Github. For example, KrakenUniq allows fast metagenomics classification using unique k-mer counts and reduces false positive identifications. Centrifuge enables classification even on laptop computers and pairs well with portable sequencing platforms such as Oxford Nanopore devices to enable sequencing and analysis in the field. Also, Pavian is a visualization tool developed to facilitate downstream analysis of datasets. Dr. Pasour is working with the team to transition these products to Army/DoD use. In addition, a collaboration with Dr. Rob Knight and Dr. Peter Dorrestein at the University of California – San Diego (UCSD) is resulting in the sequencing of microbial genomes and characterization of metabolite produced, and Dr. Jon Clary and Dr. Gleb Pischany at Harvard Medical School have requested a subset of the isolate collection for small molecule screening.

The success of the modeling portion of this project has shown that theoretical ecology is primed to be adapted to multi-dimensional host-ecosystem interactions; key differences between traditional ecological communities and communities such as the skin microbiome in which the "habitat" (the host) is itself a living, co-evolving member of the community, and the interactions are largely cooperative (instead of predator-prey) require fundamental and novel departures from existing theory, and are evolving into a new sub-focus of the Fundamental Laws of Biology focus in the ARO Biomathematics program.

Expertise developed during this project has led to collaborations with Dr. Gene Millar (Uniformed Services University of the Health Sciences). His group is focused on the epidemiology and prevention of skin and soft tissue infections among U.S. Army Infantry trainees at Fort Benning. One of these investigations incorporated the longitudinal collection of microbiome swabs from multiple anatomic sites (nasal, pharyngeal, inguinal, perianal) over the course of the 14-week Infantry training cycle. Swabs from >600 trainees were collected. A number of skin microbiome objectives are currently being addressed: association between the host microbiome and risk of subsequent infection; impact of bicillin mass prophylaxis (for prevention of group A Strep infection) on the nasal/throat microbiome; and how cohabitation in a congregate military training environment influences host microbiome, i.e. whether the common schedule, diet, and environment of military trainees may lead to a convergence of host microbiome during the training cycle. In addition to collaborations with Dr. Millar, sequencing and analysis platforms developed on the MURI led to collaborations with Dr. Phil Karl (USARIEM) in his studies of the effects of high altitude and MRE consumption on the gut microbiome.

Computational Mathematics Program

Current Scientific Objectives

01

Develop the mathematics for models and computational methods for common themes in anomalous physics (viz. anomalous transport, exponentially accelerated fronts, non-Markovian behavior and long-range interactions, self-similarity and scaling, singular behavior, interfaces, finite-domain decorrelation effects) which are expected to enable more efficient capabilities for combustion/propulsion designs, nondestructive testing capabilities for materials, and faster/more efficient engineering design of materials for the future Army

02

Create models and computational methods for material-related issues in layered and 2D geometries, energetic crystals, and porous media, which hold promise for designing new post-silicon materials for the next generation of electronics

Program Manager

Dr. Joseph Myers
Program Manager, Computational Mathematics
Program Manager (Acting), Modeling of Complex Systems
Division Chief, Mathematical Sciences
ARO Information Sciences Directorate

Dr. Myers has served as a logistician from platoon to brigade combat team level, has served as a Combat Developments Officer, and served on the Mathematics faculty at the United States Military Academy (USMA). He holds a doctorate in Applied Mathematics from Harvard, four Master's degrees from various academic institutions, including the Industrial College of the Armed Forces, and a PE license from Indiana. After retirement from active duty, he joined ARO in 2008.

SUCCESS STORY

Making Feasible the Modeling of Many-Electron Materials for Engineering Design

This ARO initiative has led to **advances in modeling and understanding electronic states**, potentially enabling future ultra-sensitive chemical detectors and ultra-efficient miniaturized electronics.

This success supports these ARL Core Technical Competencies:

Materials and Manufacturing Sciences

Computational Sciences

Challenge

Some of the most interesting and useful materials for engineering design involve materials with many interacting electrons, with complexity generally increasing exponentially with number of electrons, and therefore are incredibly hard to accurately model for prediction and design of electronic materials and sensors and etc. The importance of density functional theory (DFT) in quantum chemistry and materials science can scarcely be overstated. For over four decades, it remains the most widely used method for describing electronic states in all manner of nanoscale phenomena, including chemical bonds in molecules, band structures of materials, electron transfer, and reactive metal clusters of proteins. By some estimates, approximately 20% of all public high performance computing (HPC) resources are devoted to DFT calculations. Its prowess lies in providing a formally exact description of the immensely complicated interacting many-electron system, in terms of an auxiliary system of non-interacting electrons, called the Kohn-Sham system. While DFT is being widely used in a range of fields, it suffers from two major limitations. Firstly, the accessible system-sizes in routine DFT calculations are limited to a few hundred atoms. This is a result of the limited parallel scalability of existing implementations, in conjunction with the cubic-scaling computational complexity in solving the governing equations in DFT. Secondly, the universal exchange-correlation functional, which encapsulates all the quantum-mechanical interactions, is not known and is modeled. This limits the accuracy of DFT calculations to, at most, systems that are weakly correlated.

Action

ARO PMs for Materials Synthesis and Processing, and Computational Mathematics held discussions with ARL material scientists, and computational scientists to investigate the feasibility of progress in this area, and to identify an academic researcher with the right background and vision to make progress. Professor Vikram Gavini was identified and engaged in discussions with the PMs and lab scientists, and the PMs decided to co-fund Professor Gavini. The initial grant made some progress and demonstrated some key advantages in the use of a real-space (rather than spectral), and finite-element basis formulation. Though these are generally viewed as complex and therefore not commonly attempted, ARO funded a follow-on effort to further develop the models in this area, accompanied by a significant computational hardware acquisition.

Result

During the initial stages of this work, in collaborations with CCDC ARL Computational and Information Sciences Directorate (CISD) and Sensors and Electron Devices Directorate (SEDD), it was demonstrated that higher-order adaptive finite element basis (adaptivity guided by error estimates) can provide an efficient discretization of the Kohn-Sham equations (governing equations in DFT), and can indeed serve as an alternative to the widely used plane-wave discretization among systematically convergent basis sets.

Building on this, Gavini's group has developed efficient and reduced-order scaling algorithms for the solution of the Kohn-Sham equations,

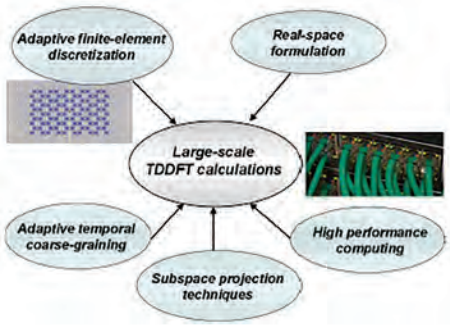


Figure 1: Overview of the technical approach. The project has developed computational techniques for large-scale Time Dependent-Density Functional Theory calculations using: (i) a real-space formulation; (ii) an adaptive finite-element basis for the discretization; (iii) an adaptive temporal discretization; (iv) subspace projection techniques; (v) massively scalable implementation on parallel computing platforms.

This success was made possible by the following ARO S&Es:

- Dr. Joseph Myers, ARO Mathematical Sciences Division
- Dr. David Stepp, ARO Engineering Sciences Directorate

Results

- Research results accepted for publication in *Nature Communications*
- Selected as one of two finalists for the *2019 ACM Gordon Bell Prize* for outstanding achievement in High Performance Computing

which also include tuning the algorithms to maximize the parallel scalability and reduce time to solution. This includes important details such as mixed precision ideas, taking advantage of GPU acceleration, and strategies to reduce data movement costs. Based on these advances, an open source code development project was undertaken in 2016 with the first beta release of the DFT-Finite Element (FE) code (https://github.com/dftfeDevelopers/dftfe) in August 2018. Some highlights of this DFT-FE code include: (i) capability to simulate system sizes of the order of 100,000 electrons (to chemical accuracy), treating metallic, insulating, periodic and non-periodic systems on an equal footing; (ii) scalability demonstrated on up to ~200,000 central processing units (CPUs) and ~22,000 graphics processing units (GPUs); (iii) significant outperformance of widely used DFT codes in both wall-clock time and CPU time (on both periodic and non-periodic systems) when solved to similar accuracy; and (iv) the ability to handle both pseudopotential and all-electron calculations in the same framework. Based on the performance metrics of DFT-FE, which demonstrate a time-to-solution that is 9x faster than widely used codes and more than 10^{15} floating point operations per second of sustained peak performance on the Summit supercomputer. This work has been selected as one of the two finalists for the *2019 Association for Computing Machinery (ACM) Gordon Bell Prize*. The scientific significance of this work is recognized by its scheduled appearance in *Nature Communications*.

Way Ahead

Advances in these computational abilities will enable the design of new electronic materials with unprecedented electronic, optical, and chemical properties, which in turn may deliver new Army capabilities for communication, physical detection, chemical detection, geolocation, energy harvesting, and other capabilities. CCDC ARL scientists remain cognizant of the work and will receive the code when it is rewritten from research code to lab code.

SUCCESS STORY

Optimal Assignments through Perfect Graph Coloring

This ARO initiative is **advancing the Army's ability to assign complex resources nearly optimally**, such as in mapping sub-tasks to nano-states and modeling electron states in materials, thereby setting the stage for ultra-sensitive chemical detectors, powerful miniature personal electronics, and other capabilities.

This success supports these ARL Core Technical Competencies:

Network and Information Sciences

Computational Sciences

Challenge

There is a large class of important problems, including the assignment of interdependent operational tasks, the scheduling of tasks or processes, the assignment of frequencies in bandwidth management, the sequential/concurrent construction of codes, and many others, that can be abstracted and analyzed as problems in graph coloring. This involves finding a coloring of a graph, meaning an assignment of colors to the vertices (states or classes) in such a way that adjacent vertices receive different colors, with the objective of using as few colors as possible. This abstraction yields

a common structure that can then be analyzed with ideas from graph theory. The problem of finding an optimal coloring is NP-complete (the hardest class of complexity) in general, but there is a particular class of graphs, called "perfect graphs", where an optimal coloring (and therefore possible optimal networks of sequencing) can be computed much more efficiently. Finding these yields a roadmap for optimal scheduling, classification, or dependencies in these applications.

Action

In 2016, the ARO PM for Computational Mathematics was discussing with colleagues on the Mathematical Sciences faculty at USMA what is new and what might be ripe for progress in Graph Theory; graphs and especially perfect graphs were identified as an area which is highly applicable to many resource scheduling applications and where some recent progress had been made. The current PI is a world expert in this area and after some conversations about feasibility, scope, and potential relevance, she developed an ambitious proposal for addressing the most relevant questions involved, and we funded her investigations beginning in 2016.

Result

During the initial stages of this work, the focus of the investigation was solving these problems when the input graph is known to be "perfect" (i.e., is a member of a certain class of graphs which all have a highly restricted structure). The principal investigator made significant progress in this area, and then realized that those new techniques could be extended further, enabling her to solve the above problems on more diverse types of input graphs.

Building on this, the problems of computing the maximum (or maximum weight) stable set or clique, as well as the problem of graph coloring are well known questions in graph theory, and are all closely related to each other. It is also known that they are NP-complete (that is, they cannot be solved efficiently when the input is a general graph). However, often graphs that come up in real life situations are not general; they are known not to contain certain configurations or have large parts that avoid certain configurations. Such graphs often have interesting structural properties that can be used to solve the problems above.

Figure 2: A perfect graph, with coloring. There are two cliques, the largest clique number is 3, and the maximum number of colors required to color any clique is 3. Decomposition and coloring help identify how to schedule actions or resources to overlap (to minimize time or to bring all required inputs together, etc.) or to avoid overlap (to avoid destructive interference or to maximize duration of contact, etc.).

Way Ahead

This result by the PI has moved most of the community toward believing that proof of the general result is indeed possible and work toward the general proof continues. Success is likely to provide bounds on the computational complexity of guaranteed bounds for resource allocation, providing an upper bound on hardware/time/bandwidth requirements for applications, and may help inform the processing steps that can achieve minimal resource requirements. USMA and ARL scientists remain cognizant of the work and will receive the results and associated algorithms.

This success was made possible by the following ARO S&Es:

- Dr. Joseph Myers, ARO Mathematical Sciences Division

Results

- Achieved most general result to date: Color every perfect graph that does not contain "4-squares"
- Result has tipped most of community toward believing that proof of the general result is indeed possible

Modeling of Complex Systems Program

Current Scientific Objectives

01

Establish the geometric and topological foundations and mathematical analysis frameworks needed to increase the accuracy and speed of all modes of geometric-based data recognition, reconstruction, and signal classification

02

Exploit deeper topological frameworks (homological, categorical, etc.) and geometric modeling techniques which will enable new capabilities in the prediction and/or explanation of social group structure and dynamics

Program Manager

Dr. Joseph Myers

Program Manager, Computational Mathematics
Program Manager (Acting), Modeling of Complex Systems
Division Chief, Mathematical Sciences
ARO Information Sciences Directorate

Dr. Myers has served as a logistician from platoon to brigade combat team level, has served as a Combat Developments Officer, and served on the Mathematics faculty at the United States Military Academy (USMA). He holds a doctorate in Applied Mathematics from Harvard, four Master's degrees from various academic institutions, including the Industrial College of the Armed Forces, and a PE license from Indiana. After retirement from active duty, he joined ARO in 2008.

SUCCESS STORY

Machine Learning Advances Acknowledged by the Test of Time

This ARO initiative has advanced the Army's capabilities to **analyze, decompose, filter, and rebuild signal and image data**, setting the stage for future image processing capabilities such as rapid facial recognition, or sensing capabilities in the infrared regime.

Challenge

Over 10 years ago, researchers were confronted with the old problem of how to quickly decompose a matrix into its fundamental components, but in the new context of very large

This success supports these ARL Core Technical Competencies:

Materials and Manufacturing Sciences

Computational Sciences

sets of streaming data, as found in computer vision and signal processing. An additional challenge was that the ultimate objective was not to enable this capability on specialized supercomputers, but rather to run on ordinary computers so that it could be deployed on low-cost and even portable devices for use by users ranging from consumers to military teams. This question is one of the most fundamental problems in applied mathematics, computer vision, and machine learning, and it is ubiquitous in data science, e.g., for processing video data continuously collected by the Army and Department of Defense. For example, it is the central issue involved in processing images and videos to remove objects from images as illustrated in the figure, processing the left image to transform it into the right.

Figure 1: A common requirement for image processing

Action

The ARO PM for the Modeling of Complex Systems Program held discussions with ARL electronics engineers and data scientists to investigate the feasibility of progress in this area and to identify academic researchers with the right background and vision to make progress. Professor Guillermo Sapiro was identified, and ARO PM and ARL engaged in discussions that led to the funding of Professor Sapiro.

Result

This research rapidly made very good progress in uncovering algorithms for use in identification tools, with transitions to the intelligence community. The program has supported Professor Sapiro since that time and has helped connect him with ARL scientists and others working in related areas of potential application. The result has been so influential and far-reaching, that the corresponding publication received the *2019 International Conference in Machine Learning Test of Time Award*, which is given to a paper that is recognized as being instrumental in helping establish the field and remains highly cited and influential many years after publication. Leadership by helping others to increase their own knowledge, is one measure of the success of one's own work, and this award exemplifies how this scientific development was able to do so.

This success was made possible by the following ARO S&Es:

- Dr. Joseph Myers, ARO Mathematical Sciences Division

Results

- Algorithms for identification tools transitioned to U.S. government agencies
- Received the *2019 International Conference in Machine Learning Test of Time* Award
- Collaboration with ARL scientists for new capabilities in rapid identification and for use in the IR spectrum

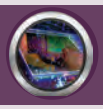
Figure 2: Combining ideas from the physiology of hand tremors with harmonic analysis and ML, Professor Sapiro's team developed an important data processing tool, the first-ever algorithm that could handle matrices with millions of components while processing the data on the fly as it arrives. It is currently available to the general public in a popular software package. A typical example is illustrated here, where the blurry image on the left is automatically enhanced to produce the sharp one on the right.

SUCCESS STORY

Topological Data Analysis for Decision-making, System Design, and Material Performance

This ARO initiative has developed a **learning algorithm for analyzing complex, multi-dimensional data in real-time to reveal previously-hidden patterns**, which will significantly enhance artificial intelligence used in navigation, human-machine interfaces, and material identification.

This success supports these ARL Core Technical Competencies:



Network and Information Sciences

Computational Sciences

This success was made possible by the following ARO S&Es:

- Dr. Joseph Myers, ARO Mathematical Sciences Division

Challenge

Analysis of large, heterogeneous data sets is complex, and often requires human intervention and categorization in order to derive some degree of understanding or insight. It has been known for some time that large data sets are typically never generated by totally random processes, there are relationships hidden in the data that can potentially be identified and exploited for greater understanding. Such topological/geometric structures that appear, and disappear, in data sets can be identified and tracked by persistence diagrams. These allow us to compare and classify structures in the data by means of statistical summaries, such as the mean or variation of persistence. However, such feature vectors are tailored to specific scientific problems, and miss or lose some of the vital information about the topology/geometry of the data space. The main reason for using such summaries is the lack of a unifying statistical framework on the space of persistence diagrams. This project has focused on applying machine learning and statistical inference directly to the space of persistence diagrams in order to make stronger assertions about the information content.

Action

In 2016, the ARO PM for the Modeling of Complex Systems program identified topological methods for feature analysis in data as a potentially productive area for real-time decision making and data sampling strategies and developed it as an element of the program's thrust efforts in data modeling and analysis. Several new investigators were contacted and either visited or engaged in correspondence, and several new principal investigators (PIs) were recruited in this area, to include Professor Bubenik, Professor Maroulas, and others. This formed a new thrust area for the program in topological data analysis. Goals were to explore statistical frameworks for estimating distributions of persistence diagrams, developing robust classification algorithms employing a statistical framework of persistence diagrams, and to apply the resulting classification algorithms to solve complex data analysis problems.

Result

PIs have worked to define a novel metric on the space of persistence diagrams in order to define what "better" means, develop a probabilistic framework on the metrized space of persistence diagrams, develop a framework for estimating the topological state of persistence diagrams, and develop state of the art, unsupervised and supervised learning algorithms using distribution theory on persistence diagrams.

Definition and Theorem

For a compact set $W \subseteq \mathbb{R}^2$, we let $P_{W,k}$ denote the set of persistence diagrams D in $W \cap \mathbb{R}^2$ with $|D| < k$. Given two persistence diagrams D_1, D_2 in $P_{W,k}$ with $|D_1| = n \leq m = |D_2|$, $D_1 = \{x_1, x_2, \dots, x_n\}$ and $D_2 = \{y_1, y_2, \dots, y_m\}$, and $c > 0$ and $1 < p < \infty$, define

$$d_p^c(D_1, D_2) = \left(\frac{1}{m}\left(\min_{\pi \in \Pi_m} \sum_{i=1}^{n} \min\left(c, \|x_i - y_{\pi(i)}\|_\infty\right)^p + c^p(m-n)\right)\right)^{1/p}.$$

Then $(P_{W,k}, d_p^c)$ is a complete, separable metric space.

- Smaller $c \Rightarrow$ more weight on matching between "small" persistence points, important for *fine* geometric differences in data.
- Larger $c \Rightarrow$ more weight on cardinality differences, important for large scale geometric differences.

Figure 3: New metric capable of identifying both fine geometric differences in data and also large scale geometric differences through adjustment of a single parameter.

Building on this, the problems of computing the maximum, or maximum weight, stable set or clique, as well as the problem of graph coloring are well known questions in graph theory, and they are all closely related to each other. It is also known that they are NP-complete meaning that they cannot be solved efficiently when the input is a general graph. However, often graphs that come up in real life situations are not general, they are known not to contain certain configurations, or have large parts that avoid certain configurations. Such graphs often have interesting structural properties that can be used in order to solve the problems above. The initial focus of the proposal was on solving these problems when the input graph is known to be "perfect," which is a certain class of graphs, all of which have a highly restricted structure. Having made significant progress in this direction, it was realized that the techniques can be extended further, to solve the above problems on more diverse types of input graphs.

Way Ahead

This research supports the Army Modernization Priorities of Soldier Lethality (shoot/don't shoot), Next Generation Combat Vehicle (human-machine interface), Long Range Precision Fires (energetic materials), and others. The researcher is coordinating with CCDC ARL HRED and Oak Ridge National Laboratory on validating and implementing these methods in Army relevant scenarios, for the analysis and design of relevant systems.

Results

- Developed methods applicable to a wide variety of decision-making scenarios, such as making instant shoot/don't shoot decisions, designing improved human-machine interfaces, and predicting chemical properties of new materials

Probability and Statistics Program

Current Scientific Objectives

01

Further develop the foundations of statistical inference in the following two ways: develop algorithms for finding many nearly optimal solutions to equations rather than just one optimal solution, and develop inferential procedures when there are several plausible models for the physical system being studied, so the conclusions we draw from data will be more robust and defensible; if successful, this research will identify alternative strategies for operators of Army systems such as convoys, communications, and fires to adapt to local and changing conditions

02

Develop statistical analyses for data types that are especially relevant to the Army, such as physiological monitoring data collected in parallel from many people performing the same activity in the same location at the same time, that if successful, commanders will have a more complete picture of the physiological state of their personnel to improve Soldier protection

03

Advance the theory of Design of Experiments for Army-specific types of experiments to make better use of scarce experimental resources that if successful in the long term, will enable tighter, faster design iterations of gun tubes and other compute-intensive systems

04

Develop approximations to and simplifications of Stochastic Hybrid Systems of equations that if successful, will enable better network control, such as load control for networked batteries and other networked resources

Program Manager

Dr. Michael Lavine

Program Manager, Probability and Statistics
Mathematical Sciences Division
ARO Information Sciences Directorate

Dr. Lavine completed his undergraduate studies at Beloit College, receiving his B.S. in Mathematics in 1974. He received a Ph.D. in Statistics from the University of Minnesota in 1987. Dr. Lavine came to ARO in 2018 as Program Manager for Probability and Statistics after a career of more than 30 years in academia.

SUCCESS STORY

Rapid Computation of Stochastic Processes in Electronic Components

ARO funded research has developed **new methods for a more reliable control of a network of systems** such as a squad of autonomous systems, or a network of batteries.

Challenge

Stochastic Hybrid Systems (SHS) are those for which the mathematical model of the physical system includes some variables that evolve continuously and others that evolve in discrete jumps. The continuous variables are typically described by Stochastic Differential Equations (SDEs) and the discrete variables by Markov Chains (MCs). An ARO funded example is a communications network subject to random connectivity interruptions and packet loss.

SHSs can be so large and complex that detailed analysis becomes prohibitively expensive. Therefore, one needs simplifications and approximations. One promising approximation technique is called "mean field." Mean field approximations are justified when a system has many interacting components and each component is affected by many others, but the individual effects of the other components can be replaced by their mean. The scientific challenge is to use mean field approximations to develop solutions to SHSs that are computationally tractable without sacrificing significant accuracy.

A second approximation is called "moment closure." In principle, SHSs can be solved for the full probability distribution of each component. But in practice we don't always need the full probability distribution; means and variances often suffice. Therefore, a possible simplification is to solve directly for low order moments and avoid the expensive calculations of full distributions. The scientific challenge is to develop direct solutions for low order moments. One way to address the challenge is through moment-closure techniques in which higher order moments are approximated as either constants or known functions of lower order moments. One PI investigates derivative-matching methods for moment closure as an alternative to Gaussian approximations when the latter are insufficiently accurate.

Action

ARO stimulated and supported two different efforts investigating the promise of SHS for modeling of processes with discrete jumps. Scientists in CCDC ARL CISD were intrigued by the potential of SHS methods for addressing processes with jump-diffusion in electronic materials, and contributed mission funds to help support an additional exploratory effort in that direction. The PM also encouraged the principal investigator (PI) to involve students in the work through our Undergraduate Research Apprenticeship Proposal, resulting in an additional student investigation in the area. The PM initiated conversations between the PI and CCDC Ground Vehicle Systems Center (GVSC), resulting in briefings and technical exchanges between the PI and GVSC scientists in October 2019, focusing on applications of SDE modeling for mobile communications.

This success supports these ARL Core Technical Competencies:

Network and Information Sciences

Computational Sciences

This success was made possible by the following ARO S&Es:

- Dr. Michael Lavine, ARO Mathematical Sciences Division

Results

- Patent for controlling battery systems for more reliable delivery of power to Army units
- Progress on approximate solutions to Stochastic Hybrid Models that will enable more reliable control of battery systems

Result

ARO funded research created several knowledge products including (1) U.S. Patent Number 10374441, "Balanced control strategies for interconnected heterogeneous battery systems in smart grid applications," (2) the paper "Modeling and characterization of neuronal synapses using stochastic hybrid systems" accepted to the Institute for Electrical and Electronics Engineers (IEEE) Conference on Decision and Control on information transfer between neurons, and (3) the paper "High-pass filtering and noise suppression in intragenic miRNA-mediated host regulation" in review at Nature Communications on buffering noise in the level of proteins within cells. These products indicate the progress being made on approximate solutions to SHS models that can be applied to problems including control and coordination of autonomous vehicles, interconnected energy systems and smart grids and battery management, and coexistence of interacting populations.

Way Ahead

ARO funded research is part of a team studying coordination and control of autonomous vehicles. Other team members include academic experts in communications and robotics, and an autonomous trucks industry expert. GVSC believes the team's efforts will be useful to GVSC's work on autonomous vehicles and invited our PIs to present their work and develop ideas for further research in October 2019. ARO will continue to solicit proposals in SHS and transition that work to GVSC and other Army research centers.

SUCCESS STORY

Optimal Assignments through Perfect Graph Coloring

ARO funded research produced the **first ever, new statistical designs for experiments of two stress factors simultaneously**, currently being used at Picatinny Arsenal, and a subsequent proposal to fund further research is currently under ARO review.

This success supports these ARL Core Technical Competencies:

Network and Information Sciences

Computational Sciences

This success was made possible by the following ARO S&Es:

- Dr. Michael Lavine, ARO Mathematical Sciences Division

Challenge

An experimental design is a plan for conducting experiments to gain the maximum information with the minimum investment of time and resources. Good designs are important when experimental units (e.g., missiles, rockets, computer simulation runs) are expensive. The relevant subfield of statistics is called Design of Experiments (DoE). An experimental design is called static when it is chosen before performing the experiment. A design is called sequential or adaptive when it adapts to data that is collected as the experiment proceeds. That is, the observations $y_1, \ldots, y_n$ at design points $x_1, \ldots, x_n$, are used to select the next design point x_{n+1}.

The challenge addressed by recent ARO DoE funding is to develop good sequential designs. The Army needs sequential designs in two settings that have not been adequately addressed. One is sensitivity testing, which is used for finding the stress

level at which an experimental unit has a response – e.g. success or failure -- with a specified probability. For example, in testing armor, one might want to know the initial velocity of the projectile that will penetrate the armor with probability 0.01 when fired from a given distance. Good designs are known for the case where there is just one stress factor. ARO's funded research addresses the challenge of finding good designs when there are two or more stress factors. The second setting is computer experiments. Static designs are common in computer experiments. ARO's funded research addresses the challenge of developing sequential designs for more complex computer experiments.

Action

The ARO PM visited GVSC to learn about their experiments with vehicles, Natick Soldier Systems Center (NSSC) to observe their experimental setup for flame retardant garments, and the U.S. Army Research Institute for Environmental Medicine (USARIEM) to learn about their studies of human performance. Dr. Lavine has also been exchanging information with Picatinny Arsenal regarding their experiments and computer simulations, and plans to visit Picatinny to learn more first hand. Dr. Lavine consulted with NSSC about their experiments with biochemical protective garments.

Results

For sensitivity testing, ARO funded PIs first conducted a simulation study to determine which one-factor designs were most promising for generalizing to two-factors. Then, the PIs used their results to propose and test the first experimental designs for two stress factors. The PIs also produced some of the first sequential designs for computer experiments, which are now being tested and improved. The results are published in *Technometrics*, a leading journal in statistics and data science. These results will lead to more efficient testing of Army models and materiel.

Way Ahead

The sequential designs coming out of ARO funded DoE research are heuristic. ARO will fund research into non-heuristic DoE principles that will lead to even better designs. Further, ARO's current DoE grants are motivated by the needs of testing programs at the CCDC Armaments Center at Picatinny Arsenal. However, there are broader DoE needs throughout the Army and other services. Therefore ARO is working with researchers from the Armaments Center to characterize common features of DoD DoE needs in order to better inform future ARO funding. The ARO PM will meet with DoD researchers at the 2020 Defense and Aerospace Test and Analysis Workshop (DATAWorks 2020) to discuss their common needs for new developments in DoE. Then the PM will engage the DoE research community in developing new experimental designs that will apply to multiple areas in the Army and other services.

Results

- These new two-factor testing designs are some of the fastest developed and transitioned to guide experiments at CCDC Armaments Center to quickly determine optimal combinations of two factors (e.g., carbon and tungsten), to enable new steel armor plates which are both strong and light
- Improved sequential experimental designs now take advantage of intermediate values in an optimal way, enabling system designs in a fraction of the time

Communications and Hybrid Networks Program

Information
Sciences
Directoriate

- Computing Sciences Division
- Mathematical Sciences Division
- **Network Sciences Division**
- Technology Integration & Outreach Division
- ARO Special Programs

Current Scientific Objectives

01

Determine the fundamental limits on the capacity and secrecy in shared wireless networks that if successful, will enable future technologies that will maximize the use of available spectrum in congested and contested environments, while ensuring secure communications

02

Develop methods for timely gathering, delivering, and processing of critical battlefield information that if successful, will enable information superiority and situational awareness for command control

03

Achieve reliable quantum networking capabilities that if successful, will enable secure and accurate sensing and communication capabilities

Program Manager

Dr. Derya Cansever

Program Manager (Acting), Communications and Hybrid Networks
Program Manager, Multi User Network Control
Network Sciences Division
ARO Information Sciences Directorate

Dr. Cansever completed his undergraduate studies at Bosphorus University, receiving his B.S. in Electrical Engineering in 1979. He trained as an Electrical and Computer Engineer at the University of Illinois at Urbana-Champaign, receiving his Ph.D. in Electrical and Computer Engineering in 1985. He came to ARO in 2017 as the Program Manager for the Communications and Hybrid Networks Program.

SUCCESS STORY

Scalable Universal Quantum Computing and Networking Using Continuous-Variable Entangled Photonic Graphs

This ARO initiative has **shown that it is feasible to generate large scale clusters of connected photons** that can be a foundation for practical photonic quantum networking that may enable a revolution in information security.

This success supports these ARL Core Technical Competencies:

Network and Information Sciences

Challenge

Quantum networking promises secure and authenticated communication capabilities in ways that are not possible in classical communications, but it requires stable quantum memories and efficient frequency conversion, which has evaded scientists' efforts to date. In this context, the use of an all photonic approach in quantum networks is appealing because: (a) photons can travel long distances without decoherence, and are the only currently viable carrier for quantum information for any long-distance application, (b) the relative ease of generating photons, and (c) the availability of mature fabrication technologies for large integrated photonic circuits. However, currently no all-photonic architectures have been successful because the two most prominent architectures for optical quantum information processing, the discrete-variable (DV) dual-rail photonic qubits proposed by Knill-Laflamme-Milburn (KLM), and the continuous-variable (CV) proposal of Gottesman-Kitaev-Preskill (GKP), suffer from the same problem: entangling gates for universal quantum computing involve probabilistic operations due to limitations of linear optics in DV, and the need for non-Gaussian operations in CV, rendering both schemes extremely resource inefficient.

Action

Quantum networking is a very promising research area, but faces tremendous challenges in the stability and short life span of its components. Dr. Cansever postulated that methods used in network science could potentially address some of these challenges. Dr. Cansever identified Professor Saikat Guha, who is a well-known quantum scientist, but who also has a significant network science background from at BBN Technologies within the ARL Network Science Collaborative Technology Alliance, to undertake a novel research effort in fault-tolerant scalable photonic quantum computing and networking to commence new work that combined the areas of network science and quantum information.

Result

Professor Guha generated insights that are crucial towards the development of an all photonic quantum network. First, he demonstrated entangled CV Gaussian clusters, which are an excellent resource for photonic quantum processing, but are not universally capable by themselves. Second, he achieved insights in DV universal cluster generation, which uses techniques from theory of complex networks (e.g., percolation, graph renormalization) for efficient cluster creation, which again by themselves are not universally capable (Figure 1). Lastly, using the using the criteria developed by Rausendorf which identifies critical values of reliability metrics for entangled cluster of photons, he demonstrated that it will be possible to determine the threshold parameters to be used in processing photons (e.g., light squeezing), such that fault-tolerant quantum operations are feasible.

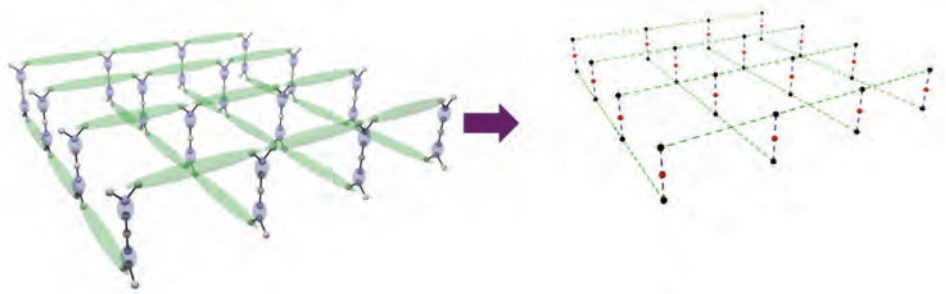


Figure 1: Creating cluster states using percolation

This success was made possible by the following ARO S&Es:

- Dr. Derya Cansever, ARO Network Sciences Division

Results

- Stable and practical scale photonic quantum networking appears to be within reach using existing technology, that may enable a revolution in information security and support remote sensing functions with previously unrealizable levels of accuracy
- Expansion of multidisciplinary research portfolios between ARO Physics and Network Sciences Divisions

Professor Guha has shown that any GKP qubit state can be prepared to 0.97 fidelity using four single-mode squeezed states (9 decibel (dB) of squeezing each), and photon-number resolving (PNR) detection of a total of 8 photons. The circuit succeeds with probability 0.001, which is a very promising result towards the goal of forming 3-photon entanglement, a basis for all photonics networking. Then, leveraging site percolation, it should be possible to generate large connected re-normalizable GKP cluster states for universal quantum computing and networking.

Way Ahead

Fault-tolerant photonic quantum computing appears to be within reach using existing (and relatively mature) technology: squeezed-light sources, linear optics, and PNR detection. The theoretical results from this short term project have kicked off a high-impact direction for fault-tolerant scalable photonic quantum computing and networking. Professor Guha will continue working towards the realization of all photonic networks and is preparing follow-on work in developing methods for multi-particle entanglement generation from GKP qubits with higher probability of success.

SUCCESS STORY

Ordering for Hypothesis Testing and Beyond

This ARO initiative has **developed the foundation needed to design and justify a different, more energy and delay efficient, distributed processing approach called ordering**, for general inference/learning/decision problems.

This success supports these ARL Core Technical Competencies:

Network and Information Sciences

This success was made possible by the following ARO S&Es:

- Dr. Robert Ulman, ARO Network Sciences Division
- Dr. Derya Cansever, ARO Network Sciences Division

Challenge

Army multi-domain operations are inherently distributed, over small and large scales, requiring communications that are timely and efficient. This will include sensor networks, autonomous agents, and Soldiers, interacting over a heterogeneous communications network, with (sometimes severe) constraints on bandwidth, energy, and computing. While there has been progress in consensus and diffusion-based distributed processing paradigms, direct incorporation of these technologies requires densely, and uniformly deployed sensors so that short range communications are always possible. The consensus and diffusion-based distributed processing paradigms also require a very large amount of these short-range communications. These result in waves of transmissions traveling back and forth across the entire deployment so that all sensors can continually iterate their decisions, such that they all agree after a time large enough to allow a sufficient number of these waves to occur. Such uniform and densely populated sensor deployments are often times unreasonable in many applications, and the excessive communications required may be energy inefficient.

Action

The previous PM for the Communications and Human Networks Program, Dr. Robert Ulman, recognized the value of efficient and secure signal processing in sensors for the Army, and engaged with Professor Blum, a well–known expert in the area. This interaction

initially led to a project regarding the Impact and Mitigation of Attacks in Sensor Networks. Subsequently, this research was extended to address distributed signal processing in sensors. Dr. Ulman has facilitated interactions with Professor Blum and ARL researchers, including Dr. Sadler, which led to very productive collaborative research activities among these parties.

Result

This collaborative research effort has developed the general theoretical underpinnings needed to design and justify a different, more energy and delay efficient distributed processing approach called ordering, for general inference/learning/decision problems that includes those with statistically dependent observations. Using such an approach in cases with statistically dependent observations, which are modeled by an underlying graph, it has been shown that; (1) it is possible to order information, and (2) that it is often unnecessary to transmit the less informative data, while retaining global optimality in the inference or decision. This results in significant savings of transmission energy and reduces decision delay, with little or no change in the error probability. It has been very recently applied to ideas in distributed learning, and shows significant improvements over existing approaches. This project has made some important advancements towards a better fundamental understanding of energy efficient distributed processing in sensor networks. This will connect Soldiers, sensors, and computing resources to enable timely access to fused sensor data to fully harness the joint capabilities of deployed sensor resources. The theories and technologies developed in this project can help the Army employ energy efficient distributed processing in sensor networks and in distributed learning/processing generally. The ordering paradigm will allow remote nodes to make decisions with minimum exchange of information to enhance target detection, surveillance, learning, inference and related tasks. The energy efficiency should significantly enhance the life of battery powered sensors and devices, while allowing compact low cost packages with a small battery payload. Figure 2 indicates the Average Number of Transmissions Saved (ANTS) due to the proposed algorithm in the research.

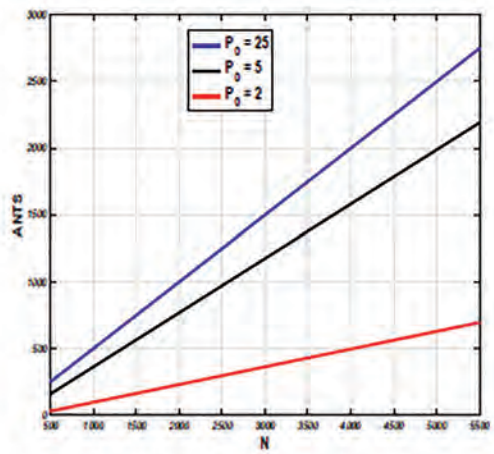


Figure 2: ANTS versus N for Different Values of Signal Powers

Way Ahead

Professor Blum will continue to develop his ideas for applying ordering to hypothesis testing, estimation and other applications. The new work will expand to new applications and extend ordering into a set of more general distributed processing approaches of interest to the Army. His studies will also extend into blockchain processing, which is relevant to the Army as the complexity of available blockchain implementations makes it unsuitable for many sensor and internet of things applications.

Results

- Co-publication between Army and academic researchers in three Institute of Electrical and Electronics Engineers (IEEE) Conferences on Signal Processing
- The graduate student of the principal investigator performed an internship at ARL
- Patent application pending

Intelligent Information Networks Program

Current Scientific Objectives

01

Model and solve imperfect information games with intermediate learning by agents that, if successful, will enable future technologies in logistics scheduling and strategy formulation in adversarial setting, with least cost to the defender and maximum cost to the adversary

02

Formalize the notion of crowdsourcing such that cognitive biases are avoided in order to utilize the power of crowds that, if successful, would lead to powerful technology for improving situational awareness of Soldiers in dense urban areas

Program Manager

Dr. Purush Iyer
Program Manager, Intelligent Information Networks
Division Chief, Network Sciences
ARO Information Sciences Directorate

Dr. Iyer completed his undergraduate studies at Indian Institute of Technology, Madras, receiving his B.S. in Civil Engineering in 1979. He trained as a Computer Scientist at the University of Utah, receiving his Ph.D. in Computer Science in 1986. He came to ARO in 2009 as the Program Manager for what was then called the Knowledge and Software Engineering, and eventually built a program in Information Networks and ultimately the ARO Network Science Division.

SUCCESS STORY

Effective Crowdsourcing

This ARO initiative led to the **discovery of principles to use suboptimal algorithms and human non-subject matter experts** to infer solutions with a high degree of accuracy, which provides a more feasible paradigm for designing future platforms relying on artificial intelligence.

Challenge

The holy grail of artificial intelligence is to create software that will act as intelligently as humans—a goal that thus far is beyond the reach of current knowledge. An intermediate challenge is to bring together human intuitions and common sense reasoning, with the

This success supports these ARL Core Technical Competencies:

Human Sciences

Network and Information Sciences

computational power of modern machines to solve problems that are too hard to solve for either one individually. The biggest challenge is to find principles to break down a problem into smaller parts that can be solved by humans (especially non-subject matter experts, using common sense), which can then be combined together by algorithms, to solve hard computational problems of interest.

Action

In 2015, Dr. Iyer pursued ideas for research in crowdsourcing as a potential source of situational awareness information. He identified many efforts that were aimed at building systems that would collect data from a large number of anonymous users (for example, Mechanical Turkers) to answer a cognitive task (e.g., label parts of a scene for machine learning applications). He found the systems-oriented approach to be less than satisfactory, as it did not answer the simple question of "to what degree can information gleaned from non-subject matter experts be trusted?" He encouraged several academics to pursue this question. As a result of his initiatives, Professor Sanjay Shakkotai, University of Texas – Austin (UTA), proposed using techniques from Queueing Theory, to take a fresh look at the question of effective crowdsourcing. Dr. Iyer brought the proposed work of Dr. Shakkotai to the attention of Dr. Brent Lance, CCDC ARL. The two decided to work together under ARL's Open Campus initiative, where one of Dr. Lance's employees spent a summer working Dr. Shakkotai's ARO funded laboratory at UTA, resulting in formalization of an optimal approach to use non-SME resources.

Result

Dr. Shakkottai, working with Drs. Brent Lance and Steven Gutstein, CCDC ARL, showed that there is a trade-off between using a small number of classifiers to obtain efficiency and using a large number of classifiers to obtain accuracy, and that this trade-off leads to a pareto-optimal strategy in resource scheduling for inference tasks. For reference, Pareto optimality is a state of allocation of resources from which it is impossible to reallocate so as to make any one individual or preference criterion better off without making at least one individual or preference criterion worse off. Indeed, the inevitability of a pareto-optimal strategy in resource scheduling for inference tasks is a result holds irrespective of ability of individual classifiers used, whether they are humans performing cognitive tasks or deep neural networks performing an inference task. The mathematical characterization leads to a scheduling algorithm, inspired by max-weight scheduling in stochastic networks, but uses a threshold based departure and maximum likelihood labeling. The algorithm achieves any point in the interior of the Pareto region without assuming any knowledge of arrival rate or classifier statistics, which can be learned using an explore-exploit strategy with a spectral estimation technique.

Way Ahead

Dr.'s Shakkottai and Lance continue to explore similar technical problems in crowdsourcing. The far term goal is for the results from the work to be adapted to the setting of a team of humans and software agents, that can collaborate on a task prescribed by a decision maker.

This success was made possible by the following ARO S&Es or Program Specialists:

- Dr. Purush Iyer, ARO Network Sciences Division

Results

- Established ongoing collaborative research among ARL Open Campus and ARO extramural researchers
- Co-publication between Army and academic researchers in prestigious International Conference on Machine Learning (ICML 2019)

SUCCESS STORY

Algorithmic Game Theory

This ARO initiative led to the demonstration of a **software agent programmed with artificial intelligence capabilities** that performed better than humans in more than 10,000 iterations of a standardized game.

This success supports these ARL Core Technical Competencies:

Human Sciences

Network and Information Sciences

This success was made possible by the following ARO S&Es or Program Specialists:

- Dr. Purush Iyer, ARO Network Sciences Division

Challenge

Since September 11, 2001, the landscape of armed conflict has changed for the U.S. Army. While it still fights large battles (such as in Afghanistan or Iraq), it is now routinely called upon to deal with asymmetric warfare against non-state actors, and sometimes rebuild societies, all under the constraint of budget and resources. Planning, strategizing, and decision making under the constraints of budget and resources, against both state and non-state actors, can always be investigated using the prism of Game Theory (as proposed by von Neumann, Morgenstern and later by Nash). However, the beautiful theoretical frameworks built in 1940s and 1950s are not that easily applicable in practice, as they do not scale well, account for imperfect information, nor account for understanding of human behavior discovered in the second half of the 20th century. Addressing these challenges will have incredible impact on the Army and society.

Action

Dr. Iyer's program supported a workshop in 2011, held at Duke University, to define what needed to be solved, and also funded a summer school for students to be trained in the burgeoning area of Algorithmic Game Theory at Carnegie Mellon University, held the summer of 2012. During that time, he published a Multi-disciplinary University Research Initiative (MURI) topic inviting proposals in this area, and promoted Dr. Vince Conitzer as an ideal candidate for the Presidential Early Career Award. Building on the success of the MURI that began in FY11, led by Professor Tambe, Dr. Iyer wrote a MURI topic in FY18 based on Network Games that reason at a societal level, and a MURI topic in 2019 on Unified Decision Theory to model human biases and its impact on decisions made by large groups. In parallel, he used single investigator funds to support Professor Tuomas Sandholm to extend Game Theory to other arenas such as interactions at the cellular level between the immune system and cancer cells.

Results

During FY19, Professor Sandholm, working with a biologist, made advances in formulating interactions between pathogens and the human immune system. This ongoing work treats the problem as an imperfect information game due, to the lack of complete knowledge of cellular level interactions. The formulation leads to a state space that turns out to be incredibly large. Professor Sandholm has made advances in designing abstractions of these state spaces so that all of the game tree does not need to be constructed in memory, but represented to allow for the reasoning effect that a sub-tree represents to maintain its influence on the rest of the game. While these abstraction techniques are still being explored in the biological domain, the author tested it on a simple game with great results. Professor Sandholm was able to reason about state space as large as 1,023 states, and conducted

Results

- Demonstration of a software agent programmed with artificial intelligence capabilities that performed better than humans in more than 10,000 iterations of a standardized game
- Research results published in *Science* (DOI: 10.1126/science.aay2400)

experiments to show that his abstraction techniques to computation of winning strategies in his software agent, Pluribus, worked significantly better than humans over 10,000 games. The results appeared in the August 30, 2019 issue of *Science*.

Way Ahead

The author is now working with Army scientists at CCDC C5ISR to understand how game theoretic techniques can be brought to bear on electronic warfare problems to protect spectrum, especially in future Multi-Domain Operations.

Multi User Network Control Program

Current Scientific Objectives

01

Determine fundamental limits of, and develop methods for, distributed control in large networked systems that if successful, will support efficient implementations of the Army's goal of distributed mission control, without losing sight of the common goal that drives its operations

02

Develop methods for learning in networked control systems, such as multi-agent reinforcement learning that if successful, will drastically enhance the operational capabilities of Army's autonomous systems, and protect the Soldiers from high-risk environments

03

Develop control methods that ensure the stability of quantum systems such as reliable qubits that if successful, will enable quantum computations that can have transformative effects such as breaking previously unbreakable codes and solving optimizations problems of unprecedented scales

Program Manager

Dr. Derya Cansever

Program Manager, Multi User Network Control
Program Manager (Acting), Communications and Hybrid Networks
Network Sciences Division
ARO Information Sciences Directorate

Dr. Cansever completed his undergraduate studies at Bosphorus University, receiving his B.S. in Electrical Engineering in 1979. He trained as an Electrical and Computer Engineer at the University of Illinois – Urbana-Champaign, receiving his Ph.D. in Electrical and Computer Engineering in 1985. He came to ARO in 2017 as the Acting Program Manager for the Communications and Hybrid Networks Program and is currently the Program Manager for the Multi User Network Control Program.

SUCCESS STORY

Time-Varying Actuation and Interconnection In Network Systems

This ARO initiative has demonstrated how the **changes in networks over time can be used to identify the causes of specific variations in the network**, thereby providing a method for understanding and repairing networks, ranging from treatments for traumatic brain injury to the design of more efficient communication systems.

This success supports these ARL Core Technical Competencies:

Network and Information Sciences

This success was made possible by the following ARO S&Es or Program Specialists:

- Dr. Derya Cansever, ARO Network Sciences Division

Challenge

Many networked systems of interest are time-varying, which creates challenges in establishing efficient control mechanisms. In fact, the state of the art in network control relies predominantly on a passive viewpoint of the time-varying nature of complex networks, where time-varying topologies are considered a given fact that needs to be dealt with. Instead, an ideal approach would be to view the time-varying interconnections and actuations as an opportunity to understand the reasons behind specific network changes and to actively shape the functionality of the system.

Action

ARO scientists recognized the value of time varying and interconnection of networked systems for the Army, and encouraged the development of several projects in this area. Professor Jorje Cortes was encouraged to submit proposal in this program area, which led to a successful project on the design and operation of time varying multi-agent networks. Dr. Cansever met with Dr. Cortes in 2019 and discussed networks found in human brains, and the underlying mechanisms used in their control. This research topic has the potential to further inspire novel control mechanisms in networked systems. This research aims to characterize the benefits and limitations of time-varying actuation (actuating different nodes at different times), and time-varying interconnection (activating different edges at different times) in time varying interconnected systems, with applications in the use of novel electrical brain stimulation schemes to treat neurological disorders.

Result

Professor Jorge Cortes and his students analyzed the potential benefits of time-varying control actuation and the role that network structure plays in it. They addressed two key questions: whether time-varying control provides any improvement over time-invariant actuation and, if so, how large the relative improvement in network controllability is, and how does it depend on its structure. For discrete-time linear dynamics evolving over directed networks, they have identified a new notion of nodal centrality, termed 2k-communicability, which measures the centrality of each node in the network at different spatial scales, defined as the maximum topological distance between pairs of nodes that allows them to affect the centrality of each other, where topological distance between a pair of nodes refers to the minimum number of edges in the graph of the network that should be traversed to go from one to the other. For instance, the spatial scale of degree centrality is 1, while the spatial scale of eigenvector centrality is infinity. Based on the distinction between local and

Results

- Best Student Paper Award, IEEE Conference on Decision and Control, Miami Beach, Florida, 2019
- Potential methodologies in addressing brain disorders such as post-traumatic stress disorder

global nodal centralities (i.e., centralities with small and large spatial scales, respectively), they have shown that the optimal control node at every time instance is the node with the largest centrality at the appropriate scale (i.e., the node with the largest 2k-communicability at an appropriate k). Accordingly, their main conclusion is that the benefit of time-varying control is directly related to the scale heterogeneity of central nodes in the network: the most benefit is gained in networks where the highest centrality is attained by various nodes at different spatial scales, while this benefit starts to decay as fewer nodes dominate the network at all scales (i.e., scale-homogeneity). As shown in Figure 1, dark points indicate the maximum level of controllability in the networks, and they increase as a function of the Time Varying Control Schedules.

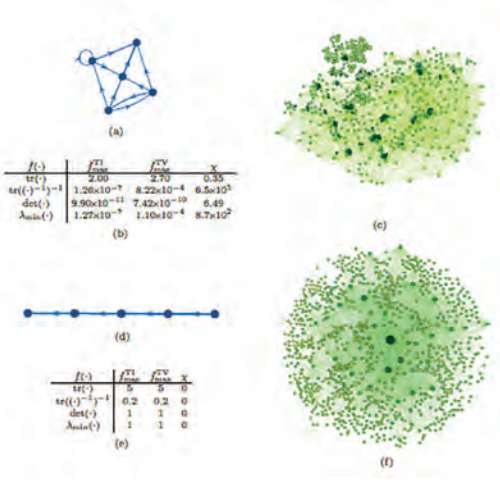


Figure 1: Illustration of the Advantages of Time Varying Control Schedules

They have also studied the problem of determining the relative importance of specific edges in the network, as a precursor to our study on time-varying interconnection. They have proposed a novel energy-based edge centrality measure using the controllability and observability Gramians, which is computationally inexpensive to compute. They have established the relationship between the proposed edge centrality measure and the gradient of the trace of the controllability Gramian. On the basis of this relationship, existing or potentially new edges can be ranked in descending order of their centrality measure as a proxy for their relative impact on the network controllability properties. Building on this notion, they have devised a computationally efficient network modification algorithm by first selecting a small subset of edges with the largest centrality measures and then maximizing the trace of controllability Gramian over the selected subset. The latter step, which is in general computationally expensive, is feasible due to the small size of the selected subset of edges and can be solved using publicly available software.

Way Ahead

Future research will compare the effectiveness of model-based and data-driven control schemes for the treatment of epilepsy and other neural diseases. If successful, this is expected to transition to the Army Medical Research and Development Command, Walter Reed Army Institute of Research (MRDC-WRAIR) to develop methods for the diagnosis and control of combat related brain disorders.

SUCCESS STORY

Computational Methods For Large-Scale Interconnected Systems With Continuous And Discrete Parameters

This ARO initiative revealed **mathematical methods for analyzing and improving problem-solving algorithms**, that may lead to advances in artificial intelligence.

This success supports these ARL Core Technical Competencies:

Network and Information Sciences

This success was made possible by the following ARO S&Es or Program Specialists:

- Dr. Derya Cansever, ARO Network Sciences Division

Challenge

Nonconvex optimization is at the crux of most of the real-world problems. For example, the nation-wide optimal power scheduling problem in electrical systems, also known as optimal power flow problem, can be cast as a nonconvex quadratically-constrained quadratic programming problem, where the nonconvexity stems from the underlying laws of physics. The nonconvexity is also inherent to most of the problems in machine learning, from the classical compressive sensing and matrix completion/sensing, to the more recent problems on the training of deep neural networks, as they often possess nonconvex landscapes. Reminiscent from the classical complexity theory, this nonconvexity is perceived to be the main contributor to the intractability of these problems. In many cases, this intractability implies that in the worst-case instances of the problem, spurious local minima exist and there is no efficient algorithm capable of escaping them. However, a lingering question remains unanswered: are these worst-case instances common in practice or do they correspond to the pathological or rare cases?

Action

A previous PM for Multi-User Network Control identified non-convex optimization problems which naturally occur in many instances, such as in machine learning and in distributed control of interconnected dynamic systems as an important research area for the Army. The PM met with Professors Oren and Lavaei in a Decision and Control Conference, which resulted in a joint ARO Project on Computational Methods for Large-scale Interconnected Systems with Continuous and Discrete Parameters, with applications in interconnected power generation systems. When Dr. Cansever visited the PIs, extensions of this research were discussed, focusing on distributed control with applications in non-convex machine learning problems. Dr. Lavaei submitted a proposal, which is currently under evaluation.

Result

The research focused on a class of nonconvex optimization problems where the input data varies over time, as in the case of large scale machine learning systems. As a motivating case study, they considered the optimal power flow problem with a California load profile, and empirically show that, despite having multiple point-wise local solutions at every time step, the local trajectories converge to the global solution over time. Inspired by this observation, they introduced the notion of spurious local trajectory as a generalization to the point-wise spurious local solutions. They showed that a time-varying optimization can have point-wise spurious local minima at every time step and yet, it can be free of spurious local trajectory. By building upon this notion, they consider a class of nonconvex optimization problems with equality constraints and model their local trajectories as an ordinary differential equation (ODE). They show that the absence of the spurious local trajectories in this time-varying optimization is equivalent to the convergence of all solutions in its corresponding ODE. Based on this equivalence, they consider a class of time-varying, univariate optimization problems, and present sufficient conditions under which, despite having point-wise spurious local minima at all times, the time-varying problem is free of spurious local trajectory. They showed that the time-varying nature of the problem is essential for the absence of spurious local trajectories. The outcome of

Results

- Best Paper Award Finalist for American Control Conference, 2019
- Uncovered mathematical methods for analyzing and improving problem-solving algorithms, that may lead to advances in artificial intelligence

this research is significant in that it provides a fundamentally sound analysis of the behavior of many local optima in learning systems, and identifies conditions under which the many local optima of this non-convex problem stay in the neighborhood of the global optimum.

Way Ahead

Dr. Lavaei will extend spurious optima results into reinforcement learning problems. This topic is of great interest and will be presented to the ARL Distributed and Collaborative Intelligent Systems and Technology Collaborative Research Alliance.

Social and Cognitive Networks Program

Current Scientific Objectives

01

Team Science: Discover fundamental principles governing human teaming activities that support designing and maintaining high performance teams that, if successful, will reduce "gel" time for squads, platoons, staffs, and joint combat operation teams for faster deployment of more effective units while improving Soldiers' cognitive resilience

02

Computational Social Science: Create verifiable models of networked human behavior by bridging social science theories with computer science techniques and engineering precision that, if successful, will create the ability to forecast societal opinions and shifts with pin-point accuracy to support Army and Joint Operations by providing support for decision-making

Program Manager

Dr. Edward T. Palazzolo

Program Manager, Social and Cognitive Networks
Network Sciences Division
ARO Information Sciences Directorate

Dr. Palazzolo completed his undergraduate studies in 1997 at the State University of New York at Buffalo as a double major in Psychology and Communication. He received his M.A. from the State University of New York at Buffalo in Interpersonal and Organizational Communication in 1999. He earned his Ph.D. in 2003 at the University of Illinois Urbana-Champaign in Organizational Communication and Knowledge Management. He came to ARO in 2014 as the Program Manager for the Social and Cognitive Networks Program.

This success supports these ARL Core Technical Competencies:

Human Sciences

Network and Information Sciences

This success was made possible by the following ARO S&Es:

- Dr. Edward T. Palazzolo, ARO Network Sciences Division

SUCCESS STORY

Building a Novel Basic Research Program for Mind-Body-Community Connections

This ARO initiative **set the trajectory for the scientific community to engage in interdisciplinary basic research** that will bring together social scientists with neuroscientists, create mathematical models linking social networks with neural networks, and will uncover the underlying relationships between the layers as well as the ability of mindfulness and hypnosis to facilitate such relationships.

Challenge

The scientific community is only beginning to understand how the mind-body is coupled at the intersection of biology and psychology. There are no clear, coherent models pushing beyond the mind-body connection. Specifically, there is a need to understand how one's social network influences his/her cognitive network, which in turn influences his or her neural network, and vice versa. That is, can we establish a scientific theory describing how the people someone connects with and the messages received change the way they think? And how does the way people think, change the way their brains are wired? In turn, how does the way people's brains are wired influence the way they think, and influence the people they choose to spend time with, and the messages they choose to consume?

Action

In 2015 Dr. Palazzolo began building a research program around the idea of "Mind-Body-Community Connections," to bring together his backgrounds in psychology, communication, social networks, and knowledge management (i.e., Social and Cognitive Networks), with the next level to include neuroscience. Additionally, he wanted to pull in his personal passion for mindfulness and hypnotherapy as potential force multipliers for managing and improving the cognitive dimension and, thereby, the individual's overall wellbeing. With this vision in mind, he teamed up with Dr. Fred Gregory, ARO's Program Manager for Neurocognition (Life Sciences Division). Together, they successfully authored and competed a Multidisciplinary University Research Initiative (MURI) topic, and secured funding for a research team comprised of four interdisciplinary scholars from the University of Pennsylvania (UPenn), the University of North Carolina at Chapel Hill, and Columbia University. The Mind-Body-Community (MBC) MURI team hosted their kickoff meeting in FY19 at UPenn with government representatives from CCDC ARL ARO, CCDC ARL, Army Research Institute (ARI), and the Training and Doctrine Command (TRADOC). During this one-day kickoff meeting, the MBC MURI team presented their vision for the five year research effort in significantly greater detail than possible in their proposal. Figure 1 shows the timeline of the research overlaid with their research thrusts. Figure 2 depicts the premise of the research towards building an MBC Model to explain behavioral choices for drinking.

The government team provide feedback that led to restructuring parts of the project and completely cutting out the hypnosis components. This strategic restructuring allowed the researchers greater resources and ability to focus on building the foundational work for a model of how the mind, body, and community are interdependently connected.

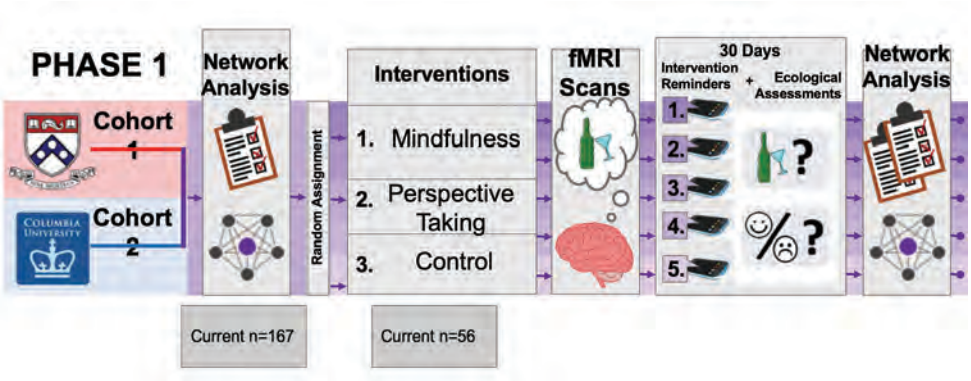


Figure 1: Outline of MBC research timeline and thrusts

Figure 2: Research Premise: Examining interactions between brain network dynamics and social network variables to predict cognitive, physiological, and behavioral choices

Simultaneously in FY19, within the Social and Cognitive Networks portfolio, ARO PM initiated a two year, standalone hypnosis research effort to offset some of the high risk associated with the MBC MURI and allow for more focused research within each team.

Result

The MBC MURI team responded to the government team's feedback and tightened up their longitudinal experimental design. Throughout FY19, their first year of the program, the MBC team got approval for conducting human subjects research and effectively recruited and engaged 167 participants in this study. All participants were randomly assigned to experimental conditions where some received mindfulness training and others did not; all participants are following an Ecological Momentary Assessment protocol for tracking their thoughts around drinking and mapping their social network throughout the day. Additionally, 56 of the participants, took part in baseline function magnetic resonance imaging scans for mapping the brain regions associated with specific thought patterns and social network priming.

Results

- ARO initiated a new research program to discover the ways people's minds, bodies, and social networks are interconnected.
- An Army Community of Interest has been created around this topic including basic scientists, applied researchers, and practitioners at Walter Reed Medical Center and Boston VA Hospital; all with particular interest in mindfulness and hypnotherapy.
- The academic team established research protocols, received approval for human subjects data collection, and have begun collecting data with participants at two universities.

The Columbia based hypnosis team, comprised of a social scientist and a clinical hypnotherapist as principle investigators, and five Ph.D. students and three Postdocs, worked closely with the MBC MURI team. In FY19, they established their protocols and recruitment strategies, and are in the process of getting human subjects' approval for data collection. Specifically, the focus of this research program is on determining and understanding the underlying mechanisms associated with hypnotherapy. This is not clinical research; that will follow with other Army research elements under the medical command. If successful, the theories, models, and results of this two year program will feedback into years four and five of the MBC MURI team's work.

Way Ahead

If successful, these combined programs will provide transformational scientific discoveries with respect to the interdependencies of the mind, the body, and social networks and messaging. Moreover, developing better models and scientific understanding of the way hypnotherapy and mindfulness can help warfighters more quickly recover from post-traumatic stress disorder (PTSD), return home, and reintegrate with their communities. Additionally, this work extends to survivors of psychological traumas of all kinds.

Although both efforts are early in their development, these two programs are attracting significant attention from multiple government agencies and research teams including ARL, Veteran's Affairs in Boston, Walter Reed Medical Center, TRADOC, and ARI. Ultimately, the goal is that this work will contribute to building significantly greater cognitive resilience in warfighters such that they are able to avoid developing PTSD symptoms all together.

SUCCESS STORY

Computational Social Science as a Tool for Counterterrorism

ARO funded research published in the Proceedings of the National Academy of Sciences (PNAS) revealed **game-theory models can be used as predictors for repeat and reactionary terrorist activity.**

This success supports these ARL Core Technical Competencies:

Human Sciences

Network and Information Sciences

Computational Sciences

Challenge

The U.S. Government and many non-profits collect copious amounts of data about terrorist activities. Although useful for situational awareness and statistics reporting, this data does not inherently provide the predictive capabilities necessary to counter terrorism. Social science theories and methodologies can be harnessed to provide meaning from the vast data, but studies in this area have been severely lacking.

Action

A principal thrust of the Social and Cognitive Networks (SCN) program is focused on Computational Social Science (CSS) to create verifiable models of networked human

behavior by bridging social science theories with computer science techniques, mathematical modeling, and engineering precision. Dr. Palazzolo seeks to bring the power of CSS to problems of significant importance to the Army and Joint Operations.

Dr. Palazzolo worked with a mathematics professor at California State University – Northridge, Professor Maria D'Orsogna, who specializes in developing mathematical models of human social systems with a Game Theory lens, particularly with respect to criminal gangs and gang violence. Her grant, funded in FY16 focuses on developing network science models to characterize the network structure of new immigrants, the back-and-forth interaction between host population and immigrants, and the network causes for youth radicalization. In FY17, Dr. Palazzolo coordinated meetings for Dr. D'Orsogna to brief CCDC ARL scientists and share her latest mathematical models of both immigrant and criminal behavior.

Dr. Palazzolo enabled Professor D'Orsogna to work with Army Scientists and apply her skills and techniques to national defense challenges. She chose the Global Terrorism Database (GTD) for source data to analyze and worked with ARL postdoc Dr. Noam Ben-Ascher, whom she met at her FY17 talks. The GTD is a catalog of global terror attacks from January 01, 1970 to December 31, 2017. Professor D'Orsogna's research focused on attacks from 2014 [when al-Qaeda (AQ) disavowed the Islamic State in Iraq and Syria (ISIS)] through 2017. Comparisons of these data are shown in Figure 3.

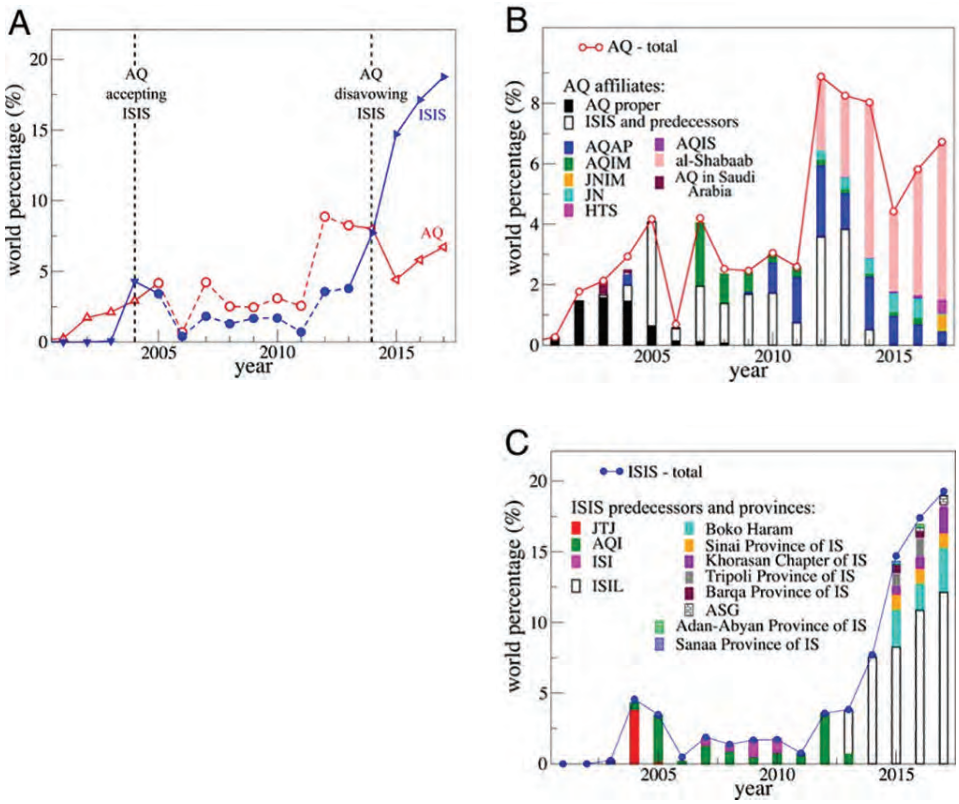


Figure 3: (A) Percentage of world terrorist attacks from 2000-2012 attributed to AQ and ISIS; (B) Percentage of terrorist attacks attributed to AQ from 2000-2018; (C) Percentage of terror attacks attributed to ISIS from 2000-2018.

This success was made possible by the following ARO S&Es:

- Dr. Edward T. Palazzolo, ARO Network Sciences Division

Results

- Discovery of method to predict probability and location of subsequent attacks following insurgent activities
- Published in the Proceedings of the National Academy of Sciences (PNAS)
- Data shared with intelligence analysts at the Training and Doctrine Command

Results

The research team analyzed the GTD dataset using near-repeat analysis tools, developed for criminology, to assess the probabilities of events happening within a fixed time window and fixed geospatial distance apart. Their analyses revealed that subsequent attacks within a 20km radius of an initial attack are more likely to occur within a four week timeframe for AQ and within a 10 week timeframe for ISIS. This elevated probability of subsequent attacks reduces for both AQ and ISIS when the distance is greater than 100km from an attack, for all time windows.

Leveraging another criminology tool based on game theory models, the research team conducted near-reaction activity analyses between AQ or ISIS (global organizations), and smaller terrorist groups (local organizations) such as the Taliban in Afghan-Pakistan region, and Houthi in Yemen. The research results show smaller terrorist groups promptly respond to an attack by AQ or ISIS, while AQ and ISIS are much slower to respond to an attack by smaller groups.

These findings in terrorist activities are similar to patterns found in urban crime, though their parameters are a little different. In urban crime, the critical zones for repeat attacks are two to six weeks (contrast here to four to 10 weeks), and a few hundred meters (contrast to 20km). Professor D'Orsogna speculates these larger windows (time and distance) with terrorist activities as compared to urban crime, is a result of the larger impact of the types of attacks. Likewise, in urban crimes, smaller gangs need to retaliate more quickly after an attack to demonstrate they have not lost any ground whereas larger gangs can respond more slowly, typically with a more calculated and targeted attack.

Way Ahead

This work was published in the Proceedings of the National Academy of Sciences (PNAS) and has been shared with intelligence analysts at the Training and Doctrine Command. They will be able to incorporate both the near-repeat event probabilities and the group size near-reaction activity into their training environments. Additionally, this research has been shared with network scientists in ARL for continued coordination with Professor D'Orsogna and additional analyses.

Education Outreach Program

Current Scientific Objectives

01

Introduce students to the Army's interest and investment in science and engineering research through associated educational outreach efforts, supporting the preparation of students for the 21st century workforce

02

Through Army funded apprenticeships, provide hands-on research experience for high school and undergraduate students, anticipated to lead to student career exploration and promote interest in STEM fields of study

03

Grow the scale of high-quality mentorship experiences for students who will benefit from the expertise of world-class scientists and engineers as a mentor for professional and academic development

04

Coordinate selection of and engagement with National Defense Science and Engineering Graduate (NDSEG) Fellows to maximize potential contribution to the defense research ecosystem

Program Manager

Ms. Jennifer Ardouin

Program Specialist, Education Outreach

Technology Integration and Outreach Division

ARO Information Sciences Directorate

Ms. Ardouin completed her Bachelor of Science degree in psychology from the University of Maryland, European Division, Heidelberg, Germany in 1991 and earned a master's degree in Industrial and Organizational Psychology from Capella University, Minneapolis, Minnesota in 2004. Ms. Ardouin pursued her career interests through active duty U.S. Army service and state and federal government service. She came to ARO in June 2017 as Program Manager of the Army's High School Apprenticeship Program (HSAP), the Undergraduate Apprenticeship Program (URAP), and various other STEM outreach activities.

SUCCESS STORY

Inclusion of Community College Students in the 2019 URAP

Information
Sciences
Directoriate

- Computing Sciences Division
- Mathematical Sciences Division
- Network Sciences Division
- **Technology Integration & Outreach Division**
- ARO Special Programs

This success supports these ARL Core Technical Competencies:

Human Sciences

This success was made possible by the following ARO S&Es:

- Dr. Stephanie McElhinny, ARO Life Sciences Division
- Ms. Jennifer Ardouin, ARO Technology Integration & Outreach Division

ARO's support of this initiative resulted in the **inclusion of community college students in the Army's Undergraduate Research Apprenticeship Program**, potentially expanding URAP to increase diversity among our Nation's STEM literate citizenry.

Challenge

According to a report from the Whitehouse Committee on science, technology, engineering, mathematics (STEM) Education of the National Science & Technology Council, 2018, "establishing a path to basic STEM literacy for all Americans is vital to preparing the diverse workforce needed for the United States to lead and prosper in an increasingly competitive world driven by advanced technology." However, a wide body of literature lays out that there is not only a lack of representation in STEM degree programs and occupations along racial and ethnic lines, but also along those of gender, disability, socio-economic status, and military veterans. While this evidence indicates that a diverse and STEM literate workforce is critical to our Nation's future global competitiveness and leadership, currently not all Americans have equal access to STEM education, or are equally represented in STEM occupations. Similarly, diversity in educational outreach participation in the Army's Undergraduate Research Apprenticeship Program (URAP) in 2019 included 37% female, 5% Black or African American, 15% Hispanic or Latino, 0% as Native Hawaiian or other Pacific Islander, and 4% as Other, with 0% identifying as military veterans.

Action

Prior to the 2019 apprenticeship request for proposal deadline, Dr. Maria Napoli, Institute for Collaborative Biotechnologies (ICB) team member from the University of California – Santa Barbara (UCSB), and Ms. Ardouin began discussing the feasibility of including non-traditional community college (CC) students in the FY19 URAP. Traditionally, the applicant pool and those selected for URAP placement are enrolled in a four-year college or university. However, actively soliciting students from the CC population would permit undergraduate-level students who typically lack opportunities to engage in hands-on scientific research in a laboratory setting, to apply for the URAP. Initially, Ms. Ardouin suggested pursing support through funding from the Army's Education Outreach Program (AEOP) Strategic Outreach Initiative, which is available to STEM partners to expand access and participation of students in existing AEOP programs. However, due to restrictions around the use of that funding, the proposed project was not selected. After consulting with the AEOP Consortium to ensure there were no restrictions cited by the cooperative agreement or DoD policy, Ms. Ardouin approached Dr. Stephanie McElhinny, the ARO PM monitoring the ICB University Affiliated Research Center (UARC), at the time. Dr. McElhinny supported the proposed efforts, pending her evaluation and approval of UCSB's written FY19 URAP proposal.

UCSB later submitted the required URAP proposal in accordance with the ARO Broad Agency Announcement and the proposal was approved for funding. Upon notification of proposal acceptance, UCSB leveraged their previously established relationships with CCs within a 100 mile radius of their campus, of which many were Hispanic Serving Institutions (HSIs). UCSB directly disseminated printed and electronic information to the Mathematics Engineering Science Achievement (MESA) chapters and Veteran Education Counselors throughout their CC network, to market and solicit applications for the 2019 URAP opportunity. Based on UCSB's knowledge of area demographics, the marketing efforts targeted a fairly large population of underrepresented, underserved students and military veterans.

Result

UCSB successfully recruited three CC students and each was paired with junior level, near-peer UCSB undergraduate students, all of whom participated in hands on research in three laboratories on the UCSB campus. Apprentices participated in research projects titled; "DASA-based Photochromic Materials for Load-bearing Applications: Emulating Nature's Design to Build Light-addressable Actuators," "Global States and Cognitive Priority Control," and "Engineering Sense-and-Respond Enzyme Complexes for Bioproduction".

This story is evidence of indirectly removing a barrier that may have existed for CC students who wished to access active research laboratories, engage with world class Army funded researchers as mentors and benefit from near –peer experiences with four-year undergraduates and other members of the principal investigator's (PI) research team. In addition to CC students gaining invaluable research experiences, UCSB URAP PIs provided additional activities which included URAP participants receiving training to develop and enhance their scientific presentation and communication skills, opportunities for STEM career exploration, and STEM ethics training.

During a site visit to UCSB, Ms. Ardouin was able to attend URAP students' poster sessions, tour each of the three laboratories, hear presentations from the student pairs, and provide an overview of other Army and DoD STEM educational opportunities (Figure 1).

Figure 1: UCSB URAP Students.

While AEOP specifically, and DoD generally, have implemented broad initiatives to increase access to STEM opportunities to those who are underserved and under-represented, this effort at UCSB was a small but key step in expanding the STEM pipeline. It did so by introducing CC level students to the apprenticeship opportunities, supporting them in applying for such programs, and exposing selected students to laboratory fundamentals through hands-on research and other skills that are beneficial as part of a larger STEM workforce development program.

Way Ahead

The potential Army impact of supporting this initiative may serve as a model for other university partners participating in the URAP, who wish to engage in a similar outreach efforts to CC students.

SUCCESS STORY

ARO Leverages Army Assets In Support Of Local STEM Outreach Event For Underrepresented And Underserved Students

This success supports these ARL Core Technical Competencies:

Human Sciences

This success was made possible by the following ARO S&Es or Program Specialists:

- Ms. Christine Doss, Administrative Officer
- Ms. Jennifer Ardouin, ARO Technology Integration & Outreach Division

ARO and CCDC Soldier Center partnered to **introduce the science and engineering used to create the Meal Ready-to-Eat (MRE) for 150 underrepresented minorities, girls, and low-income middle and high school students**, exposing them to the results of Army research.

Challenge

ARO often collaborates with Research Triangle Park (RTP) STEM a local STEM outreach organization whose mission is to expose underserved and underrepresented middle and high school students to STEM professionals who serve as short term mentors, and an array of STEM educational opportunities. RTP STEM hosts three STEM themed festivals each year, inviting more than 150 students from schools across North Carolina. ARO is often invited to participate in the session of the STEM Fest that involves a hands-on demonstration of research or what a STEM professional might do during a typical day at work. Being that ARO is not an active laboratory but rather an extramural funding organization, it has been a challenge to provide age appropriate demonstrations for this group.

During past STEM Fests, ARO PMs have demonstrated exciting aspects of Army research, such as technologies designed to protect military working dogs while in a deployed or field environment. However, in an effort to provide a broad view of Army research and not overtax the small number of scientific staff at ARO, there was a need to leverage other Army research assets for these outreach events.

While education outreach events are administered and managed by the education outreach program manager, successful participation in such events are staff intensive and often require the support of a broad spectrum of ARO scientific program managers, non-scientific program managers, administrative, and computer support staff members.

Action

In attempt to identify another interactive and age appropriate demonstration for students attending the STEM Fest, Ms. Ardouin met with Ms. Christine Doss, who has a long history of supporting ARO's educational outreach efforts to brainstorm possibilities. Together they developed an idea around the observation that during past STEM Fests, students seemed particularly interested in Meals Ready to Eat (MREs) that were displayed as props in the Army research booth. They consulted with other ARO staff, Mr. Rich Freed and Mr. John Stone, who provided us with contact information for staff at CCDC Soldier Center in Natick, MA.

After an array of planning conference calls and coordination, demonstrators Ms. Priscilla (P.J.) Bitopoulos and Ms. Patricia (Patty) Cariveau, both from the Combat

Feeding Directorate of CCDC Soldier Center committed to traveling to ARO to partner with us to engage Fest attendees.

During the event; ARO staff participated in the speed mentoring, Ms. Ardouin and Ms. Doss provided attendees and their teachers with printed information and answered questions regarding educational opportunities available through the Army Education Outreach Program (AEOP), while Bitopoulos and Cariveau discussed the research, science and engineering involved in every aspect of the MRE contents and container, including the design of the flameless ration heater, packaging the meals to ensure meals extended shelf life, and that they are highly portable and ergonomically designed to fit into cargo pockets of military uniforms. Students were given an opportunity to taste samples of many of the MRE items (Figures 2-4).

As an added bonus and after the STEM Fest, Ms. Bitopoulos and Ms. Cariveau provided an update to a group of ARO staff and guests from the RTP Foundation on the latest in MRE science and technology. After the briefing, attendees participated in a question and answer, and tasting of the newest MRE offerings.

(Clockwise) Figure 2: ARO Speed Mentors, **Figure 3:** MRE Staff briefing, **Figure 4:** MRE Science Featured at STEM Fest

Way Ahead

ARO staff will continue partnerships with the RTP STEM to reach NC's underrepresented population by representing Army research at quarterly STEM festivals, as well as partnering with other local STEM outreach organizations. Such partnerships will introduce others to the Army's investment in research and commitment to STEM education outreach to students, in an effort to fortify our Nation's future STEM savvy citizenry.

Department of the Army STTR Program

Current Scientific Objectives

Since 1992, the Congressionally-mandated STTR program has provided Army-wide research and development opportunities for small business/research institution partnerships, with $37.4M in funding in FY19. The Army STTR Program is diversified across all ARL core competencies (average funding percentages): Materials/Manufacturing Sciences (24%), Computational Sciences (10%), Ballistics Sciences (3%), Human Sciences (3%), Propulsion Sciences (8%), Network and Information Sciences (27%), and Protection Sciences (11%).
Other investment areas include Biomedical, Nuclear, and Space platforms

01

Army STTR investment portfolios are aligned with the Army Futures Command (AFC) Modernization Priorities and CFTs that have identified S&T needs, and other AFC mission areas, such as the Army Application Laboratory (AAL) *Capability Accelerator*, which helps small businesses and universities mature concepts into prototypes and validate early-stage technology at Capital Factory, Austin, TX

02

Army STTR is also focusing projects to post-prototyping/venture capital initiatives such as *Army Strategic Capital* and the *UTDD* as a transition-bridging partner for all innovative STTR prototypes prior to fielding/sustaining with warfighting commands

Program Manager

Mr. Michael John Smith

Program Manager, Department of the Army STTR program
Technology Integration and Outreach Division
ARO Information Sciences Directorate

Mr. Smith completed his B.S. in General Engineering at the United States Air Force Academy, Colorado Springs CO in 1987 and his MBA at West Coast University, Los Angeles CA in 1994. He came to ARO in 2018 as the Program Manager for the Army's Small Business Technology Transfer (STTR) program. Previously, he was the Army Small Business Innovative Research (SBIR) Program Manager from 2010 to 2017.

SUCCESS STORY

Army STTR Special Topics and Industry Day

Army STTR teamed with U.S. Army Special Operations Command (USASOC) to pilot a **rapid-response, prototyping-transition program**, bringing innovative technologies direct to the warfighter.

Challenge

The Army STTR program, authorized by Section 638 of Title 15, United States Code, has historically prescribed life cycle durations driven by maximum contract award periods of performance, and provided no authority to invest program funds in post-prototyping activities. Congress, the Small Business Administration (SBA), and Office of the Secretary of Defense (OSD) challenged federal STTR program managers to drastically reduce the life cycle to transition innovative technologies into fielded warfighter systems.

Action

Army STTR program office developed a pilot program to pursue rapid prototyping and transition of innovative technologies through small business and research institution partnerships to address a wide variety of warfighter capabilities in several S&T ARL core competencies. This pilot supports the ARL Core Competency, "Network and Information

TABLE 1

All Army-wide STTR investments of FY19 funding, with sub-investments associated with Industry Day indicated in green.

Organization	Number of Topics	Number of Ph 1 Projects ($M)	Number of Ph 2 Projects ($M)	Total FY19 STTR Investments ($M)
CCDC – Aviation and Missile Center	1	2 ($0.33)	1 ($1.1)	$1.43
CCDC – Armaments Center	1	2 ($0.33)	1 ($1.1)	$1.43
CCDC- Army Research Lab (ARL) / ARO	6	13 ($2.16)	19 ($15.6)	$17.76
Army Research Office (ARO) & USASOC	7	16 ($2.66)	7 ($7.70)	$10.36
CCDC – C5ISR Center	1	2 ($0.33)	2 ($2.2)	$2.53
CCDC – Chem Bio Center	2	5 ($0.83)	1 ($1.1)	$1.93
Corps of Engineers – ERDC	1	2 ($0.33)	0 ($0.0)	$0.33
Medical Research & Development Command (MRDC)	1	3 ($0.50)	0 ($0.0)	$0.50
CCDC – Soldier Center	1	2 ($0.33)	0 ($0.0)	$0.33
CCDC – Ground Vehicle and Systems Center	2	5 ($0.83)	0 ($0.0)	$0.83
FY19 TOTAL	23	52 ($8.65)	31 ($28.75)	$37.4

This success supports these ARL Core Technical Competencies:

Network and Information Sciences

This success was made possible by the following ARO S&Es and Program Specialists:

- Dr. Randy A. Zachery, Director, Information Sciences Directorate
- Mr. Michael Caccuitto, Chief, Technology Integration & Outreach Division
- Mr. Michael John Smith, Technology Integration & Outreach Division
- Ms. Nicole Fox, Technology Integration & Outreach Division
- Dr. Derya Cansever, Network Sciences Division
- Dr. Joe Qiu, Electronics Division
- Dr. Michael Gerhold, Electronics Division
- Dr. James Harvey, Electronics Division

Sciences" but will be expanded to support all ARL core technical competencies. This ARO and USASOC partnership involves all phases of the research and development life cycle processes: requirement generation, vendor selection, prototype delivery, follow-on testing, and procurement/sustainment. On 10 September 2019, ARO and USASOC co-hosted an Industry Day, allowing small businesses and universities from across the nation to learn more about these special topics written to address a warfighter need, as well as provide a forum for partnerships to form among the Industry Day participants. The event was produced with support from Virginia Tech Applied Research Corporation (VT-ARC) under a Partnership Intermediary Agreement (PIA) with ARL. VT-ARC, with support from its subcontractors, also conducted targeted outreach to small businesses and academia in technical areas most relevant to the topics advertised. This led to the generation of stronger proposals and more innovative ideas/solutions.

Result

This pilot program will invest up to $10M in STTR Phase 1 and Phase 2 pilot projects in subsequent fiscal years, and compress the Army STTR topic-to-transition life cycle from six years to two years, a 67% schedule reduction; resulting in rapid prototyping, testing, and initial fielding by 2021.

Way Ahead

The ARO PM will look into expanding the pilot's Industry Day life cycle processes to the entire Army STTR program, and address all ARL core competencies and Cross Functional Teams (CFTs), for rapid prototyping and post-prototyping activities integration with Army Strategic Capital and University Technology Development Division (UTDD).

SUCCESS STORY

STTR Phase 3 – Big Open-Source Social Science (BOSSS)

This success supports these ARL Core Technical Competencies:

Human Sciences

Network and Information Sciences

Challenge

Developing reliable human landscape situational awareness (SA) is a lengthy, often fraught process. While social scientists offer insights into human populations, their methods are designed for in-depth analyses of social structure and behaviors, and are hamstrung by outmoded research methods that do not scale to U.S. military operational engagements. On the other hand, computer and information sciences offer methods to efficiently collect, process, and organize large amounts of data, but lack a theoretical framework for evaluating the quality or the meaning of this data. As a result, troops often enter an Area of Operation (AO) with only a rudimentary understanding of the human landscape. Further, the SA that units gain while in theater is not readily passed-on when they hand over operations to the next deploying unit, requiring the new unit to develop their human landscape SA from scratch.

Action

The U.S. Army Corps of Engineers (USACE) awarded an initial $88K STTR Phase 3 to Boston Fusion, to integrate the BOSSS platform across the Army and the Department of Defense

(DoD). BOSSS provides the U.S. military with rapid and reliable SA of the human landscape – the social structures, beliefs, values, persons of influence, behaviors, economy, military, politics, and other 'hot topics' – for their AO. BOSSS structures and organizes data by applying state-of-the-art search, natural language processing, and data association techniques to rapidly search, retrieve, process and transform data into frameworks for social understanding, grounded in well-founded social science theory. BOSSS can automatically generate an initial social awareness overview for an area in a matter of hours, enabling analysts to analyze, refine and better understand the operational environment (OE). The overview currently places open source information into categories that include OE factors [political, military, economic, social, information, infrastructure (PMESII)], civil considerations [areas, structures, capabilities, organizations, people, events (ASCOPE)], and an interactive graph network with key groups and influential people. These interfaces are informed by feedback from intelligence analysts (Army Intelligence Center, 101st Airborne, Asymmetric Warfare Group), Civil Affairs, and Information Operations stakeholders. This allows BOSSS to generate a social awareness picture in a matter of hours, rather than the months that are currently required. BOSSS will transition into existing applications, such as the Distributed Common Ground Station (DCGS-A), Map-Based Planning Services (MBPS)/Joint Planning Services (JPS), and Marine Civil Information Management System (MARCIMS).

Result

BOSSS vastly improves existing extraction, processing and modeling of key groups, events, issues, and concerns in an AO. BOSSS improves operational design and planning, support analysis of civil considerations and open sources, and yields missions that more thoroughly consider key issues of integrated campaigning and the information environment. Information is an Army Capability of Combat Power and the BOSSS capability can assist commanders in understanding information impact on adversaries and neutral/friendly populations. BOSSS also supports Army requirements in the Maneuver Center of Excellence and Soldier Lethality CFT to gauge effects on combat power of non-kinetic effects such as information operations. The Synthetic Training Environment CFT requires real-time rendering that includes human terrain information, and the Intelligence Center of Excellence requires modeling, simulation and visualization of threat and non-threat behavior and events, patterns of life and potential courses of action provided by the BOSSS emerging capabilities.

Way Ahead

Because BOSSS is an emerging capability for multiple, existing DoD systems to collect information, analyze and understand operating environments, as well as conduct planning and mission command activities from the information gathered, this initial Phase 3 is focused on the detailed requirements and interfaces to integrate BOSSS across DoD. Once the interfaces are identified and implemented, further BOSSS Phase 3 awards are anticipated.

This success was made possible by the following ARO Management S&Es or Program Specialists:

- Mr. Michael Smith, Technology Integration & Outreach Division

Historically Black Colleges and Universities (HBCU) and Minority-Serving Institutions (MSI) Program

Current Scientific Objectives

01

Expand participation of HBCUs/MSIs in ARO Core research programs through innovative outreach and program design/execution

02

Enhance capacity of HBCUs/MSIs to compete effectively for ARO research grants

03

Provide outreach and research experiences to faculty and students at HBCUs/MSIs to increase awareness of Army research, partnerships, innovation, and career opportunities

Program Manager

Ms. Patricia Huff

Program Specialist, Historically Black Colleges and Universities (HBCU) and Minority-Serving Institutions (MSI)
Technology Integration and Outreach Division
ARO Information Sciences Directorate

Ms. Huff is a graduate of Howard University receiving her B.A. degree in Broadcast Management in 1987. Her professional activities and accreditations include: Master Certified Facilitator and Moderator (Qualitative Researcher). Prior to joining ARO in 2012, Ms. Huff worked for more than a decade in the federal government at the National Oceanic and Atmospheric Administration. She went on to work as a Marketing Research Analyst for Potomac Electric Power Company and later became the owner and Chief Executive Officer of a marketing and communications consulting company.

SUCCESS STORY

CCDC ARL and ARO Holds First HBCU/MSI Undergraduate Student Design Competition

ARO initiatives successfully s**howcased talent and educational prowess being developed at HBCUs and MSIs across the United States.** Talent is everywhere and this competition inspired the next generation of highly competent STEM professionals to develop solutions to real-world challenges faced by today's warfighter.

Challenge

The Department of Defense (DoD) and Army recognize that engagement from HBCUs/MSIs is critical to ensuring a diverse talent pool of researchers and students. These institutions can provide high quality faculty to perform research, and high quality students that can contribute to DoD research and engineering via internships, fellowships, and even employment.

Action

In FY19, ARO executed the first HBCU/MSI Undergraduate Student Design Competition. The ARO Program Manager, in coordination with ARL, drafted and posted the funding announcement, facilitated the proposal evaluations, and assisted in the execution of the competition in El Paso, TX in April 2019. All internal and external parties were proactively engaged to effectively and efficiently disseminate competition requirements, process and evaluate white paper submissions, and accomplish program goals with a constrained budget and against an expedited timeline. ARO worked with internal and external stakeholders to coordinate competition activities with Army's subject matter experts, Army Futures Command, and Army Contracting Command to showcase the HBCU/MSI student researchers. The inaugural year of the competition focused on unmanned aerial vehicle (UAV) technology gaps in two topic areas. The first challenged students to eliminate wire bundles in an innovative way in small UAVs and the second topic sought a way to replace UAV parts with biologically-based materials.

The competition also engaged HBCU/MSI students with the Army's technical and operational communities so that they could get a better understanding of current and future UAV capabilities, as well as Army operations, and Army science and technology. Science and engineering talent and capability lie at the heart of the Army's ability to field the World's most advanced and capable ground fighting forces. To maintain overmatch capabilities, it is vital that the Army attract students from a wide variety of academic and personal backgrounds to ensure it stays on the forefront of discovery and innovation.

Result

Five teams from HBCUs and six from MSIs were selected to participate in the competition in El Paso, TX on 23-25 April 2019. Each team received an $8,000 grant to cover travel costs to El Paso for the poster session and flight demonstration. $500 could be used to build a UAV prototype. Mentors from ARL and other CCDC centers helped students refine their design and ensure their UAV was flight worthy. More than 1,000 local El Paso middle and high school students were present and watched on as the

This success supports these ARL Core Technical Competencies:

Propulsion Sciences

Ballistics Sciences

Human Sciences

Protection Sciences

Network and Information Sciences

Materials and Manufacturing Sciences

Computational Sciences

Results

- 11 teams from five HBCUs and six MSIs were selected as finalists. The four winning teams from this event received cash prizes ranging from $5k to $2k to continue their scientific and innovative basic research academic endeavors.
- Over 1,000 local middle and high school students were challenged and inspired to pursue science, technology, engineering, and math programs to find real-world solutions to complex challenges the Army faces. These students were introduced to opportunities offered by the Army including scholarships, internships, and careers serving the nation.

competitors used their 10-minute flight block to maneuver their UAV through a series of challenges on the course at the campus of University of Texas – El Paso. These students were also exposed to different exhibitors from ARL and other Army centers to bring awareness of all of the Army science and technology programs.

The top four winning teams of the inaugural HBCU/MSI Design Competition represented the following colleges and universities:

1st Place: InterAmerican University of Puerto Rico

2nd Place: University of Texas - El Paso

3rd Place: University of Illinois - Chicago

4th Place: Spelman College

The remaining 7 team finalists who competed in the inaugural HBCU/MSI Design Competition represented Grambling State University, North Carolina A&T State University, Tuskegee University, University of Maryland - Eastern Shore, University of Puerto Rico – Mayaguez, University of Texas at Arlington, and University of Texas at San Antonio.

Way Ahead

ARO PM will execute the event on behalf of Army Futures Command and CCDC with a two day event in Chicago, IL in April 2020. The event will be hosted by University of Illinois – Chicago. This event will build upon the previous competition to incorporate lessons learned and feedback from all participants.

This success supports these ARL Core Technical Competencies:

Propulsion Sciences

Ballistics Sciences

Human Sciences

Protection Sciences

Network and Information Sciences

Materials and Manufacturing Sciences

Computational Sciences

SUCCESS STORY

ARO Hosts DoD Workshop For Historically Black Colleges And Universities (HBCUs) And Minority-Serving Institutions (MSIs)

This collaboration between the Office of the Under Secretary of Defense for Research and Engineering (OUSD (R&E)) and CCDC ARL ARO better **enabled HBCU/MSI community stakeholders to develop sustainable relationships between ARO and HBCUs/MSIs**, while creating pathways to better engage ARO's scientific community to support innovative research conducted at HBCUs/MSIs.

Challenge

The Army needs to build a stronger research network in the Historically Black Colleges and Universities (HBCUs) and Minority-Serving Institutions (MSIs) academic community that leads to a better understanding of our research opportunities, the ability to share best practices and lessons learned, and make data-driven recommendations for program improvements. The ongoing challenge is to create an interactive, informative, and engaging strategy to expand the competitiveness and research capacity at HBCUs/MSIs, and provide an opportunity for this academic community to gain a better understanding of DoD funding opportunities, priorities, and processes, to become more competitive for these opportunities.

Action

On 12-13 Jun 2019, ARO, in partnership with OUSD (R&E), hosted a two day workshop in Research Triangle Park, NC to provide technical assistance on how to do business with DoD and ARO. This year's annual workshop moved to a new two day itinerary and a new larger meeting space, to meet the demand of registrants. The interactive and engaging workshop, incorporated dedicated networking breaks and a poster exhibition of DoD HBCU/MSI Centers of Excellence's research. This expanded format enabled key stakeholders in the HBCU/MSI community to engage with technical Program Managers and subject matter experts, from across DoD, to help develop a greater knowledge of how to partner with federal agencies, how to work with DoD contracting officers (pre-award to post-award), and enhancing HBCU/MSI competitiveness beyond targeted programs. The workshop focused on increasing HBCU/MSI participation in activities throughout the DoD research enterprise, white paper and proposal processes, and highlighting what evaluators consider when reviewing proposals.

Result

This event was attended by over 225 registered participants from across the country. Participants from academic leadership and researchers, to sponsored program officials, received assistance in developing competitive proposals in response to DoD funding opportunities including the: Defense University Research Instrumentation Program (DURIP); the Multidisciplinary University Research Initiative (MURI); Minerva Initiative; Established Programs to Stimulate Competitive Research (EPSCOR); Defense Established Programs to Stimulate Competitive Research (DEPSCOR); and the Science, Mathematics and Research for Transformation (SMART) Program.

The knowledge gained from the breakout sessions, interactions with the DoD Program Managers, ARL and ARO leadership, and Army Contracting Command increased the awareness of the many DoD opportunities available to the HBCUs/MSIs and their students. This event was also supported by other federal partner agencies such as the Air Force Office of Scientific Research (AFOSR), Office of Naval Research (ONR), ARL Office of Small Business Programs, Air Force Research Laboratory (AFRL), National Science Foundation (NSF), National Aeronautics and Space Administration (NASA), and the National Academy of Sciences (NAS).

Way Ahead

ARO will continue to engage with the HBCU/MSI community to further develop areas of shared scientific interests to bolster HBCU/MSI participation in DoD funding and research opportunities.

Results

- Increased awareness of DoD research opportunities and special programs for HBCUs/MSIs
- Targeted sessions to provide feedback from proposal evaluators to ensure the HBCUs/MSIs community understands what is needed for a competitive proposal submission

ARO SBIR and STTR Programs

Information
Sciences
Directoriate

- Computing Sciences Division
- Mathematical Sciences Division
- Network Sciences Division
- Technology Integration & Outreach Division
- **ARO Special Programs**

ARO Small Business Innovation Research (SBIR) and Small Business Technology Transfer (STTR) Programs

ARO participates in SBIR and STTR Programs, and is the lead for the Department of the Army's STTR Program. The overarching goals of the SBIR and STTR programs are: (1) stimulate technological innovation, (2) increase small business participation in federal R&D, (3) increase private sector commercialization of technology developed through federal R&D, and (4) foster and encourage participation in federal R&D by businesses that are owned by women and socially and economically disadvantaged individuals. The STTR Program has the additional requirement that small companies must partner with an academic or other qualifying non-profit research institutions to work collaboratively to develop and transition emerging technical ideas from the laboratory to the marketplace. In FY19, ARO awarded $39 million in SBIR and STTR contracts.

Program Manager

Ms. Nicole R. Fox

Program Specialist, Small Business Innovation Research (SBIR) and Small Business Technology Transfer (STTR)
ARO Technology Integration and Outreach Division

Ms. Fox completed her B.A. in Business Administration at Bay Path University in 1997. She came to ARO in 2010 as a contracted Program Specialist for the Army STTR program and joined federal service as the ARO SBIR/STTR Program Specialist in 2011.

SUCCESS STORY

REAPR - Innovative ES/EA Suite Extends to Airborne Platforms

This ARO small business and academic partnership resulted in the **discovery and development of a ground-based, remotely-controlled, intelligent, electronic attack system** known as Reactive Electronic Attack Portable Radio (REAPR) that is ready for transition to an Army Program of Record.

Challenge

America's current electronic warfare (EW) capabilities are insufficient for the modern and future battlefield. In order to safeguard against radio-controlled threats and disrupt enemy communications, current EW systems clash with friendly force systems within the electromagnetic spectrum (EMS). Current systems require large power sources and generate distinct radio frequency (RF) footprints that can be easily tracked and located by adversaries. The size weight and power (SWaP) profiles of these systems are too large for dismounted Soldiers, and their substantial RF footprints put our warfighters at risk from adversary RF tracking systems. The challenge is to provide capable training equipment to adequately prepare our warfighters for the congested and contested EMS in the battlefield, while potential adversaries are publicly demonstrating advanced EW capabilities that could cripple warfighter effectiveness if training platforms and procedures are not improved. A need for a low-cost, scalable, open-architecture, networked, intelligent jammer for warfighter training and dismounted operations support has been recognized by the Army. The Shadow aircraft's relatively small size and payload capacity present significant challenges to most electronic attack (EA) platforms.

Action

In the year 2014, Dr. Robert Ulman developed an Army STTR topic on EMS Monitor & Broadcast Training Capacity Enhancement. The topic went forward and was subsequently awarded to two STTR Phase I proposals to Kerberos International, Inc. and Intelligent Automation, Inc. Both small businesses submitted a Phase II proposal and Kerberos, with its research institution partner, Southwest Research Institute (SwRI), was selected to continue further R&D in the areas of low-cost, scalable, open-architecture, networked intelligent jammer for warfighter training and dismounted operations support.

This STTR project resulted in the development of Kerberos' Reactive Electronic Attack Portable Radio (REAPR®), a ground-based electronic attack system. Due to continued successes, Kerberos was awarded a subsequent phase II contract to advance the EW system to significantly reduce SWaP and add a geolocation capability. Due to the successful development of the REAPR and through the collaboration of Joint EW Center (JEWC), who helped conceive the topic and acted as SMEs as well as a transition partner, Kerberos was awarded a Rapid Innovation Fund (RIF) contract in 2019 for $3M to further commercialize and transition the REAPR technology. Ms. Fox served as co-Contracting Officer's Representative (COR) with Dr. Ulman on the contract, and Kerberos's Dr. Sammy Smith served as the principal investigator.

Result

The REAPR is a man-portable, networked, Commercial Off the Shelf (COTS)-based, open-architecture prototype system for providing electronic warfare support (ES) and electronic warfare capabilities (Figure 1). REAPR offers an extensible platform designed to defeat current waveforms with open interfaces and modular components so additional techniques can quickly be incorporated as new threats emerge. Upon detecting a target signal of interest (SOI), REAPR transmits an extremely precise signal designed to jam the SOI with minimal disruption to Blue Force communications, and a very small RF footprint that is not easily tracked by the enemy.

REAPR is currently a ground-based, Technology Readiness Level (TRL) 7, networked, remotely controlled, intelligent, small SWaP, ES/EA system that was initially funded by

This success supports these ARL Core Technical Competencies:

Ballistics Sciences

Protection Sciences

Network and Information Sciences

Computational Sciences

This success was made possible by the following ARO S&Es and Program Specialists:

- Dr. Robert Ulman, ARO Network Sciences Division
- Ms. Nicole Fox, ARO Technology Integration and Outreach Division

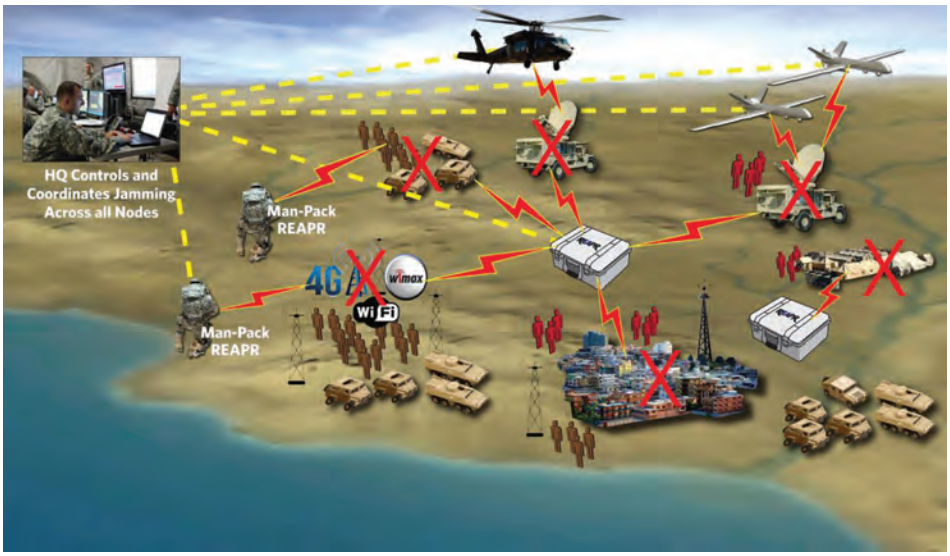


Figure 1: Conceptual illustration, REAPR, Pods to showcase the SWaP challenges, and Shadow

Results

- Demonstration of electronic signal disruption system, transitioned for use in various DoD UAS technologies
- Very small RF footprint that is not easily detected by adversaries
- Energy Efficient UAS ES/EA for the dismounted Soldier
- Reduces Cost by utilizing a widely deployed UAV platform

an STTR Phase II contract from CCDC ARL. Kerberos' first commercialization of the REAPR is through the Rapid Innovation Fund (RIF) project to adapt it from ground-based operations to a widely deployed unmanned aircraft system (UAS). REAPR offers an extensible platform designed to defeat current waveforms with open interfaces and modular components so additional techniques can quickly be incorporated as new threats emerge. An intuitive HQApp enables end users to operate the REAPR system either locally or remotely, selecting signals or frequencies of interest to target, as well as operational modes, frequency ranges, and other mission-specific data.

This research has also led to the discovery of an innovative, open-architecture ES/EA system that is capable of identifying and targeting/ jamming single channel adversary RF signals/transmissions with minimum disruption to Blue Force or commercial communications systems.

Way Ahead

The potential Army impact of this research is to repackage the current REAPR for airborne platforms and incorporate a TRL9 Time Difference of Arrival (TDOA) geolocation solution for ground and airborne platforms. The result will be a TRL8, production ready, multimode ES/EA system that emits a minimal power and RF footprint; is available on land-based and two representative airborne platforms, and is ready to transition into an Army Program of Record. If successful, Kerberos will deliver outstanding value in an innovative, airborne reactive jamming and surveillance platform. This will provide unprecedented support to forward-deployed warfighter units. The REAPR that results from this will be demonstrated to operate effectively on UAS and will be ready to start certification into programs of interest.

SUCCESS STORY

Scalable Manufacturing of Graphite Yarn via Wet Spinning Process

ARO funded researchers developed a **novel yarn supercapacitor system**, which is superior to other yarn supercapacitors reported in literature due to the elimination of a traditional textile substrate made of natural or synthetic polymers, resulting in higher density and resilience.

Challenge

New high-performance electronic and "smart" textile technologies with advanced functionalities (e.g., sensing, physical actuation) are being developed, although many functional applications are limited by the availability of low cost integrated energy storage technologies. Scalable, inexpensive manufacturing processes that produce yarns capable of storing energy are required for new breakthroughs within the wearable electronics sector. In addition to energy storage, functional yarns must also be knitted and woven into comfortable/wearable materials that are capable of wicking moisture and allowing full range of motion in ways that are similar to common athletic wear. Other desirable attributes for textile-based energy storage are that the technology solution(s) should be electrochemically stable, charge and discharge rapidly, and maintain requisite power density for thousands of duty cycles and/or for the life of the garment. To produce the requisite amount of functional yarn, manufacturing processes must be capable of producing kilometers of energy storage yarns that maintain desirable mechanical attributes both for knitting/weaving and, ultimately, yield sufficient yardage of wearable textile materials to be relevant for implementation. Finally, the energy storage technology should not leach toxic chemicals (e.g., electrolytes, or nanomaterials such as carbon nanotubes) during normal wear, nor during laundering of fabrics. Furthermore, gentle laundering should not disable the energy storage device.

In 2017, Dr. Robert Mantz developed an Army STTR topic on Scalable Manufacturing of Functional Yarns for Textile-based Energy Storage. The topic went forward and was successfully awarded three STTR Phase I proposals, of which, Storagenergy Technologies, Inc. was a selectee. All three small businesses submitted a Phase II proposal and Storagenergy Technologies, Inc. was again selected to continue further R&D in the areas of low capacitance density; low power density; low abrasion resistance (fall off); and limited scalability. With Ms. Fox as co-COR along with Dr. Mantz and Dr. Feng Zhao as the PI, the effort has been successful in the areas of mass production of MXene, multi-nozzle spinnerets (50 spinnerets) to scale up the production of GO&MXene fibers (813 km), continuous sizing of Storagenergy's Yarns, high capacitance (>50 mF/cm) of yarn supercapacitors, and improved flexibility and crumpling stability for machine weaving and knitting capabilities of Storagenery's functional yarns.

Result

The effort developed an integrated production line that can continuously produce GO&MXene yarn electrodes at a reasonable speed via the combination of multi-nozzle fiber extrusion, coagulation, collection, washing, chemical reduction, twisting, sizing, and electrolyte mediation processes (Figure 2). This effort discovered an innovative platform that can automatically derive fabrication protocols for specialized yarn/fabric products

This success supports these ARL Core Technical Competencies:

Protection Sciences

Materials and Manufacturing Sciences

Propulsion Sciences

This success was made possible by the following ARO Management S&Es or Program Specialists:

- Dr. Robert Mantz, ARO Chemical Sciences Division
- Ms. Nicole Fox, ARO Technology Integration and Outreach Division

Results

- Demonstrated mass production of MXene, a new system to rapidly speed fiber production
- Demonstrated high capacitance of yarn supercapacitors
- Improved the flexibility and crumpling stability for machine weaving and knitting capabilities of our functional yarns

according to customer requirements as ordered in details (size, shape, strength, toughness, flexibility, breathability etc.). Storagenergy's yarn-based supercapacitor incorporated into military uniforms can improve Soldier survivability like the ability to wear sensors and communicate, and also increase Soldier mobility since it reduces the weight and bulkiness relative to currently fielded power sources. Supercapacitors compared to batteries, produce system advantages in biosafety, power density, and cycling stability. These yarn or fiber shaped devices can become attractive power sources for miniaturized electronic devices such as micro-robots, physiological sensors, and even implantable medical devices, since they can have small volumes and could be easily integrated into all kinds of shaped structures.

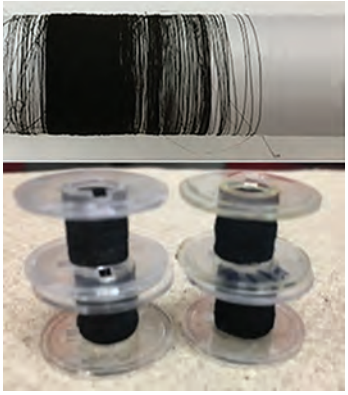


Figure 2: Conceptual illustration continuous GO&MXene fiber fabrication via a wet-spinning process

Large size 2D materials (GO&MXene) are beneficial for wet spinning good mechanical properties, especially GO materials. If pure GO was use for wet spinning, we would have the ability to develop very strong fibers. GO's capacitance is much lower than MXene, greater than 50% weight of MXene is required to reach the target specific capacitance level of 50 mF/cm. The team at Storagenergy has demonstrated a scale-up processes for MXene synthesis. The advantages of GO for yarn supercapacitors are; large size; beneficial for wet-spinning; high mechanical strength; and high electrical conductivity. The advantages of MXene for yarn supercapacitors is high electrical conductivity and high capacitance.

Storagenergy's yarn system shows (1) higher volumetric and gravimetric capacitance density, (2) higher electrical current and thus superior power density, (3) enough property retention against abrasion, rubbing, and scratching, and (4) excellent fabric flexibility and breathability. Storagenergy's team has demonstrated a scale up setup to continuously fabricate hundreds of kilometers graphene oxide (GO)/MXene supercapacitor yarns via the combination of multi-nozzle fiber fabrication and supercapacitor yarn assembly processes.

Way Ahead

The potential Army impact of this research is to develop an integrated production line that can continuously produce GO&MXene yarn electrodes at a reasonable speed via the combination of multi-nozzle fiber extrusion, coagulation, collection, washing, chemical reduction, twisting, sizing, and electrolyte mediation processes. Further, the aim is to develop an innovative platform that can automatically derive fabrication protocols for specialized yarn/fabric products according to customer requirements as ordered in details (size, shape, strength, toughness, flexibility, breathability etc.) Storagenery's yarn-based supercapacitor incorporated into military uniforms can improve Soldier survivability from the ability to wear sensors and communicate and also increase Soldier mobility since it reduces the weight and bulkiness relative to presently used power sources.

If successful, team Storagenery will develop a fabrication process of fully functional yarn based supercapacitors to be well suited for transitioning via "Smart" fabric companies to mature the interface between supercapacitor yarns and other electronic devices in a wearable system.

Electrochemistry Program

Current Scientific Objectives

01

Synthesize and characterize new electrolyte species to enable advanced power storage and generation devices that provide greater capacity and with lower weight for the Soldier

02

Understand transport in heterogeneous charged environments to allow selective control of transport of species enabling advanced sensors, protective gear, and fuel cells

03

Understand how material and morphology affect electron transfer and electro-catalysis to enable synthesis, oxidation, and reduction of Army relevant materials and energy systems

04

Explore new methods of controlling electrochemistry to enable creation of novel materials including new optical materials for rapid and resilient communication and computation capabilities for the Army network

Program Manager

Dr. Robert Mantz

Program Manager, Electrochemistry
Division Chief, Chemical Sciences Division
ARO Physical Sciences Directorate

Dr. Mantz completed his undergraduate studies at the United States Air Force Academy, receiving his B.S. in Chemistry in 1989. He received his M.S. in Chemistry for California State University, Northridge in 1994, and his Ph.D. in Chemistry from North Carolina State University in 1997. He came to ARO in 2006 as the Program Manager for Electrochemistry and was promoted to the additional role of Division Chief, Chemical Sciences Division, in 2017.

Physical Sciences Directorate

- **Chemical Sciences Division**
- Life Sciences Division
- Physics Division
- UARCs Division

SUCCESS STORY

The First Truly Versatile Polymer Electrolyte Ionomer/Membrane System

This ARO initiative resulted in the **discovery of a scalable polymer system that can be fabricated into thin robust mechanically and chemically stable films** or compatible ionomers with high ionic conductivity to enable polymer electrolyte alkaline fuel cell systems.

This success supports these ARL Core Technical Competencies:

Propulsion Sciences

Materials and Manufacturing Sciences

This success was made possible by the following ARO S&Es or Program Specialists

- Dr. Robert Mantz, ARO Chemical Sciences Division
- Dr. David Stepp, ARO Engineering Sciences Directorate

Results

- Demonstration of electronic signal disruption system, transitioned for use in various DoD UAS technologies
- Very small RF footprint that is not easily detected by adversaries
- Energy Efficient UAS ES/EA for the dismounted Soldier
- Reduces Cost by utilizing a widely deployed UAV platform

Challenge

Batteries have limited energy content. One potential solution is fuel cells which can carry an external tank of fuel and use oxygen from the air to electrochemically provide power. With fuel cells the energy content is driven by the size of the fuel tank. To date a great deal of research has been conducted on polymer electrolyte membrane (PEM) fuel cells. Perflourinated proton conducting membranes which operate under acidic conditions, such as Nafion→ (discovered in the 1960s) have sufficient performance to enable compact acid catalyzed fuel cells, electrolyzers, or sensors. Furthermore, in the Nafion→ system a variation of the same polymer that constitutes the membrane can be used as the ionomer, the ionic conductor in the electrodes. However, PEM fuel cells are limited to hydrogen and methanol as fuels. The DoD has a single fuel for the battlefield, JP-8, which is a complex hydrocarbon fuel. New fuel cell technologies beyond PEM fuel cells are required to enable use of these fuels. In contrast to proton conducting systems where the anion is always sulfonic acid, in anion conducting systems the cation can be almost any positively charged group, however, generally the conductivity of many systems is too low. Alkaline based systems have also been plagued with stability issues with a variety of degradation mechanisms leading to polymer breakdown. In contrast to proton conducting systems where the anion in the polymer is always sulfonic acid, in anion conducting systems a wide variety of cations have been attached to polymer backbones. However, usually the conductivity of many systems is too low. Alkaline based systems have also been plagued with stability issues with a variety of degradation mechanisms leading to polymer breakdown.

Action

In 2006, Dr. Mantz initiated meetings with Drs. Chu and Lundgren at ARL SEDD to determine future strategies for ARL-wide research interests in electrochemistry. Dr. Mantz recognized that the prior fifty years of research in the old Nafion→ based systems could potentially be applied to systems that operated under alkaline conditions where oxidation of fuels and reduction of oxygen are more facile. Dr. Mantz drove the launch of a workshop in 2006 bringing together the world's experts in alkaline conductive membranes and catalysts. Based on the workshop results, Drs. Mantz and Stepp wrote a 2011 MURI (multi-disciplinary university research initiative) topic on anion exchange membranes (AEM) to bring together a team of researchers with diverse expertise to attack this research which will be a critical enabler of anion fuel cells.

Drs. Mantz and Stepp strategically focused the MURI on understanding transport and stability of membranes where it was thought that physical and chemical properties such as swelling and mechanical strength could be tuned by polymer chemistry and processing. The MURI team took the approach of combining hydrocarbons backbones, which are stable under basic conditions, with cation functionalized groups. The polymers they synthesized were triblock allowing morphological control of the membrane on the nano-scale.

Result

Drs. Mantz and Stepp pushed the team to quantify the critical chemical and physical properties and the impact of processing that were needed for membranes to be practical. These properties are important because the membrane in the device must simultaneously provide a range of properties. Many other teams have emphasized

chemical stability over mechanical stability and while these films do extremely well in ex-situ external testing they perform poorly in a cell because they swell too much with liquid water or fail mechanically. Professor Coughlin sought to make new triblock co-polymers (ABA), with chemical stability, high anion conductivity, and desirable mechanical properties. Initially the team discounted the use of cyclooctene as the B part of the block copolymers because it melted at 40°C rendering the material far too weak for further study. After several iterations with Professor Herring and co-investigators a facile method was discovered to hydrogenate the B block to polyethylene. The B block was now a semi-crystalline polymer that was mechanically strong and chemically stable allowing the membrane to survive under the conditions that AEM fuel cells or electrolyzers are expected to operate in. When this polymer was quarternized with methyl pyrrolidinium cations very high ionic conductivities could be realized with low water swelling. The team was also able to expand to other combinations of monomers that allowed the team to develop ionomers for integration into device electrodes.

This new material actually shows improved mechanical properties when wet because swelling is restricted and this forces the polyethylene block to change its crystallite size. Under wet conditions the material has enhanced chemical stability superior mechanical properties, and better ionic conductivity than other materials investigated to date. Furthermore, this material set is amenable to allowing ionomer application to electrodes.

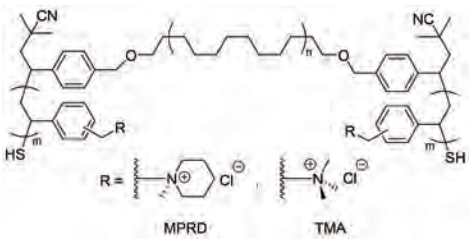


Figure 1: Molecular structures of the ABA triblock co-polymer PCMS-b-PE-b-PCMS, shown quaternized with either MPRD or TMA.

This discovery of the triblock co-polymers anion exchange membranes is the subject of a U.S. patent application and is under review for the journal *ACS Applied Polymer Materials*. The scientific article details how the mechanically stable polymer, *which was previously limited due to melting*, could be also demonstrate enhanced properties with some of the highest chloride and hydroxide conductivities ever observed.

Way Ahead

The potential Army impact of this research is in the use of these polymers to develop new fuel cells capable of using complex hydrocarbon fuels. CCDC ARL SEDD has received samples of membranes and one ionomer formulation and has evaluated bipolar membrane fuel cells which were successfully tested at temperatures as high as 80°C.

This research also led to the discovery of a new family of multi-block polymers which are scalable and have easy synthetic steps allowing for their scale up. The versatility of this system is impressive as it allows the membrane properties to be tuned but more importantly ionomers can be utilized in the electrodes, the lack of which is an Achilles heel in most other approaches. Dr. Mantz continues to invest in research to study the interaction of these polymers with metal surfaces. Future efforts will focus on using the polymer to template catalytic particles in-situ thereby realizing a complete roll to roll manufacturing process for electrochemical energy conversion devices. Commercial applications based on AEMs are still only in their infancy but this work represents an important step towards full adoption of this technology industrially.

SUCCESS STORY

Catalyst-Free Synthesis of Ammonia from Nitrogen and Water Using Plasma Electrolysis

ARO funded research led to the **first demonstration of ammonia synthesis with 100% efficiency at atmospheric pressure and temperature**, using a novel plasma electrochemistry system that required only nitrogen and water and without any catalysts, setting the stage for distributed ammonia (and similar chemical) production at forward-operating bases.

This success supports these ARL Core Technical Competencies:

Propulsion Sciences

Materials and Manufacturing Sciences

This success was made possible by the following ARO S&Es or Program Specialists:

- Dr. Robert Mantz, ARO Chemical Sciences Division

Challenge

The fixation of nitrogen in the atmosphere has a tremendous impact on energy, the environment, and society. A key process involving nitrogen fixation is the production of ammonia, which is the primary component of the fertilizers essential to agriculture. In addition, ammonia is one of the starting materials for the production of energetic materials, such as propellants and explosives. The current approach to synthesizing ammonia is the Haber-Bosch process, which requires extremely high pressures and temperatures and hydrogen gas, and thus is limited to centralized plants to take advantage of the economies of scale. This method presents a challenge for forward operating bases and tenuous supply lines. Distributed production of ammonia and similar important chemicals that can operate at atmospheric pressure and temperature and leverage renewable energy sources, such as solar or wind energy, would overcome this limitation. One possible approach that possesses these attributes is electrochemical reduction of nitrogen to ammonia in aqueous electrolytes where water serves as a source of hydrogen. However, the activation of the triple bond in nitrogen has to date been difficult to achieve by any metal electrocatalyst, leading to low ammonia yield and selectivity. Developing alternative electrolytic pathways that do not require activation of this bond on a catalytic surface is one path forward to overcoming this challenge and realizing distributed ammonia synthesis.

Action

In 2013, Dr. Mantz reviewed proposed ideas from Professor Go, University of Notre Dame (UND), to study electrochemical reactions using electrons injected into solution using a plasma. These had high potential payoff for the Army, but were extremely high risk with little to no preliminary results, so Dr. Mantz recommended funding through the STIR program to support Professor Go UND and R. Mohan Sankaran, Case Western Reserve University (CWRU), to generate initial results to support a full proposal. Their proposed work involved replacing the solid electrode in an electrochemical cell with an atmospheric-pressure plasma (also called a gas discharge), offering the potential to conduct electrochemistry without an electrode by using 'hot' plasma electrons. While Professor Sankaran had evidence that he could synthesize colloidal nanoparticles using this approach, it was unclear exactly how the chemistry worked and its potential benefit. Through the STIR, the UND and CWRU teams developed a way to directly measure that the plasma electrons solvate in the electrochemical cell and that they drive the ensuing

electrochemistry. They published the work in *Nature Communications*. This success showed the promise of this technique, leading to award of a single investigator grant and the two are advancing our understanding of plasma electrochemistry. Dr. Mantz leveraged the DURIP program to improve Dr. Go's measurement system. Using these awards, the team has made major strides in both understanding the chemistry in the system, and specifically what impacts the faradaic efficiency and selectivity, and exploring novel applications for chemical synthesis without a catalyst. This resulted in the synthesis of oxalate and formate from carbon which is a major breakthrough.

Result

This story recounts a particular success that was not a primary focus at the onset of the program, but showed how pulling an interesting intellectual thread can lead to significant findings. The primary aim of the research was to understand the nature of the plasma-solvated electron and how the plasma electrochemical environment affects its behavior and chemistry. The only application-based aspect of the program was to explore nanomaterial synthesis by reducing metal cations as a means of understanding the fundamental electrochemistry.

Professor Sankaran, however, also pursued a side project to see if he could also reduce a molecular gas similar to what Professor Go demonstrated with carbon dioxide. Using an atmospheric-pressure nitrogen (N_2) plasma in contact with an aqueous solution, Professor Sankaran was unexpectedly able to measure ammonia in the water solution (Figure 2A). Using a series of control tests, including an argon plasma, no plasma, and various pH solutions, he was able to confirm these results (Figure 2B). Further, using parametric studies Professor Sankaran demonstrated that he could synthesize the ammonia with 100% faradaic efficiency – far greater than other reported efficiencies for electrically-driven N_2 reduction to NH_3.

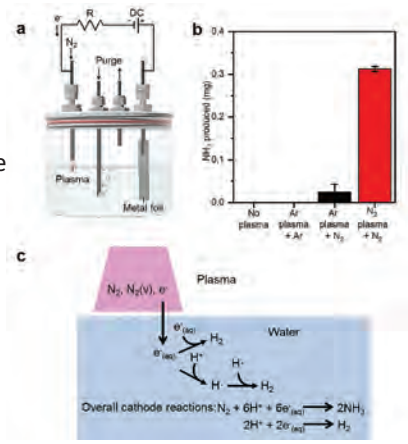


Figure 2: Catalyst-free, electrolytic NH 3 production from N2 and water using a plasma electrolytic system. (A) Schematic of the plasma electrolytic system operated by a dc power supply and galvanostatically controlled using a resistor (R) in series. The direction of electron flow (e−) is indicated. (B) Total NH3 produced after 45 min at 6 mA and pH 3.5 for various gas configurations and controls. (C) Potentially important species contained in the plasma, such as vibrationally excited N2 [N2(v)], and in the water, such as solvated electrons [e−(aq)], and their involvement in reactions, such as the generation of hydrogen radicals (H·), that lead to NH3 formation. The overall re- actions for N2 reduction to NH3 and H2 evolution (under acidic conditions) at the cathode are shown. From Hawtof et al., Sci. Adv. 2019; 5 : eaat5778 under a Creative Commons Attribution Non-Commercial License 4.0 (CC BY-NC).

These results are inherently important because they show a new approach to ammonia synthesis using nitrogen and water, as opposed to nitrogen and hydrogen. Hydrogen production from either water or a fossil fuel is inherently inefficient and limits commercial ammonia production; using pure water in plasma electrolysis not only overcomes this inherent limitation but also does so at atmospheric pressure and temperature and without requiring catalysts that can either be expensive to produce or difficult to maintain.

Through discussions with Professor Go and Dr. Bartels of UND, Professor Sankaran devised a method to determine the reaction path that leads to ammonia synthesis. Using both nitrate and nitrite to scavenge presumed intermediates, the solvated electron and hydrogen atom, it was found that solvated electrons are likely one of the driving species and that H· is also a key intermediate (Figure 2C). However, further studies are also needed to refine understanding of the reaction chemistry and hopefully reveal new ways to improve selectivity at higher current densities.

This discovery of catalyst-free plasma electrochemical ammonia synthesis was published in *Science Advances* (Hawtof et al., Sci. Adv. 2019; 5 : eaat5778, DOI:

Results

- Discoveries made possible by ARO funding and others inspired a new MURI topic (2020 MURI solicitation, Topic 17: Solution Electrochemistry without Electrodes)
- Discovery of catalyst-free plasma electrochemical ammonia synthesis was published in *Science Advances*

10.1126/sciadv.aat5778) and was featured in articles on Science Daily (https://www.sciencedaily.com/releases/2019/01/190111143731.htm) and Chemistry World (https://www.chemistryworld.com/news/lightning-inspired-method-makes-ammonia-with-no-catalyst/3009981.article) among other online science websites.

Way Ahead

Dr. Mantz is driving new ways to use electrochemistry to synthesize new nanomaterials with a myriad of applications including sensors and optical materials. It can provide access to new electrochemically generated molecules that are currently not available using traditional electrochemical techniques. This effort is complementary to in-house CCDC ARL SEDD research and CCDC ARL SEDD is participating in the review of MURI proposals to enable collaborations and technology transitions.

Environmental Chemistry Program

Current Scientific Objectives

01

Develop sensitive and selective analytical methodologies to create new unprecedented capabilities to identify chemicals in complex environments that if successful, will enable future technologies to detect the presence of explosives and toxic chemicals in real-time

02

Monitor transformations of chemical species from source to point-of-detection and predict future transformations under a range of environmental conditions that if successful, will enable source attribution to chemicals and contaminants mobilized in the environment and predict Soldier risk

03

Model chemical reaction mechanisms over a wide range of temporal and spatial timescales that if successful, will help close the gap between nanoscale chemical reactions and macroscale environmental dynamics

Program Manager

Dr. Elizabeth King

Program Manager, Environmental Chemistry
Chemical Sciences Division
ARO Physical Sciences Directorate

Dr. King completed her undergraduate studies at Boston University, receiving a B.S. in Marine Science in 2012. She trained as an environmental chemist at Oregon State University, receiving her Ph.D. in Earth, Ocean, and Atmospheric Sciences in 2017. She came to ARO in 2019 as the Program Manager for Environmental Chemistry.

SUCCESS STORY

Real-Time Ultra-Trace Detection of Organics from Environmental Matrices

ARO is driving studies to establish n**on-destructive, real-time methods to detect and quantify chemical warfare agents, toxic industrial compounds, and their degradation products** that in the long term will lead to new methods to protect the Soldier from warfare agents.

This success supports these ARL Core Technical Competencies:

Protection Sciences

Computational Sciences

This success was made possible by the following ARO S&Es or Program Specialists:

- Dr. Robert Mantz, ARO Chemical Sciences Division
- Dr. Elizabeth King, ARO Chemical Sciences Division

Challenge

The ability to detect chemicals and contaminants (e.g., chemical warfare agents and toxic industrial chemicals) in an environment is paramount when assessing hazards and implementing remediation strategies. Unfortunately, many chemical species are difficult to measure with current technologies due to their low concentrations (parts per trillion) and the presence of compounds that interfere with the signal of interest in a typical sample matrix (e.g., soil) during analysis on a mass spectrometer. Measuring chemical species in a complex matrix leads to situations where important chemical signatures are not readily apparent during analysis. New techniques must be developed to minimize the aforementioned complexities and maximize the capabilities of field-based analytical detection. This challenge is exaggerated for first responders and forensic technicians who must often selectively collect samples to extrapolate through an entire contaminated area.

Action

Beginning in 2018, the Acting Environmental Chemistry Program Manager, Dr. Mantz, recognized the novel approach proposed by Professor Brian Clowers from Washington State University to overcome trace-level detection challenges by forming selective stable chemical clusters that can then be measured in regions of the mass spectrum that are not crowded by matrix interferences.

The detection of hazardous compounds at ultra-trace levels requires developing methods that are sensitive and selective, with minimal sample preparation. Few detection modalities providing real-time sensing into the ppt range are compatible with non-contact sampling. Moreover, traditional approaches focus predominantly on sample ionization via charge transfer. This may not provide the level of selectivity needed to realize ultra-trace levels of detection because many chemicals of interest fall with the same mass-to-charge (m/z) ratio. By leveraging selective clustering reactions where two species share a charge, thus altering the m/z ratio of the stable cluster, the detection of low volatility compounds is possible using traditional ion detection techniques (i.e., mass spectrometry). Kinetic reaction atmospheric flow tube mass spectrometry (KRAFT-MS) using dielectric barrier discharge ionization has emerged as a technique that combines such features for vapor detection.

The overall concept of KRAFT-MS is based on the knowledge that a longer reaction time between analyte molecules and reactant ions enables molecules to form stable clusters that then become ionized in an m/z range free of matrix interferences. Given the extended interaction time between charged reactant ions and neutral analytes the probability of an interaction is greatly increased. When favorable, a stable, charged heterodimer can form

which is readily distinguished from background ions using mass spectrometry (Figure 1). While there is typically never a complete conversion of the analytes of interest into these stable clusters, the signal-to-noise ratio significantly decreases when the clusters sit in a different part of the mass spectrum. Therefore, the overall sensitivity of the analyte of interest increases such that it can be identified in real-time.

The optimization of KRAFT-MS requires better understanding of selective gas-phase clustering by determining the proton affinities for species of interest and selecting an optimum clustering reagent. Analyte stable clusters are possible when using a high volatility reagent ion in the presence of a low volatility. To understand clustering dynamics fundamental aspects of dissociation and association energies needed to be studied.

Result

Combining KRAFT technology with mass spectrometry provides a non-destructive, real-time method to quantify chemical warfare agents, toxic industrial compounds, and their degradation products. The major goal of this project was to characterize the kinetic routes of high-pressure ionization mechanisms that enable ultra-trace level detection schemes for a suite of chemical compounds. In order to establish proof-of-concept, Professor Clowers designed a series of experiments to identify the pathways and products of cluster formation for standard chemical warfare agents with a phosphorus functional group and their degradation products (e.g., dibutyl phosphonate, ethyl phosphonic acid, monobutyl phosphonate, methyl phosphonic acid, and tributyl phosphonate). Figure 2 outlines the experimental approach and compares the relative survival yield (SY) curves between different clusters by which their proton affinities may be deduced (Figure 2A). A qualitative comparison of proton-bound dimerization of analyte and selected reagent was also performed (Figure 2B). While this is a limited selection of phosphates and correspondingly a small set of heterodimers, some trends can still be observed (Figure 2C). For example, increasing the length of the alkyl chain attached directly to the phosphorous atom has the impact to slowly add stability to the proton-bound dimer interactions. Therefore, using these data as a guide, clustering reagents with larger alkoxy chains may serve as optimum ion clustering reagents.

Once proof-of-concept was established, computational chemistry techniques were employed to determine a suite of functional groups that can be used on unknown samples as clustering agents. At the completion of these studies, Professor Clowers created the chemical framework for a new class of analytical techniques aimed at the real-time detection of analytes relevant to the mission of the ARO (e.g., CWA degradation products, decontamination solvents, and common groundwater contaminants).

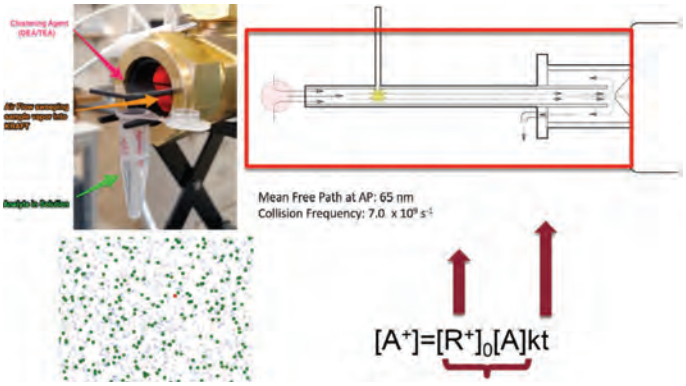


Figure 1: Analytes detected by KRAFT-MS are from non-equilibrium vapor concentrations only. The top picture shows analyte and dopant introduction into the atmospheric flow tube. The time spent in the tube will maximize the probability that a cluster forms which can be detected. The equation shows which kinetic elements improve with flow tube optimal residence time. The red square is the analyte, the green circles are the dopant clustering ion, and the gray circles are background gas.

Results

- Co-publication between Pacific Northwest National Laboratory and academic researchers in the journal *Analytical Chemistry*
- Academic researcher hired by Pacific Northwest National Laboratory to provide in-house expertise in recently-developed mass spectrometry technologies
- Collaboration between academic researchers and Smiths Detection using KRAFT-MS technology as a detection mechanism for narcotics

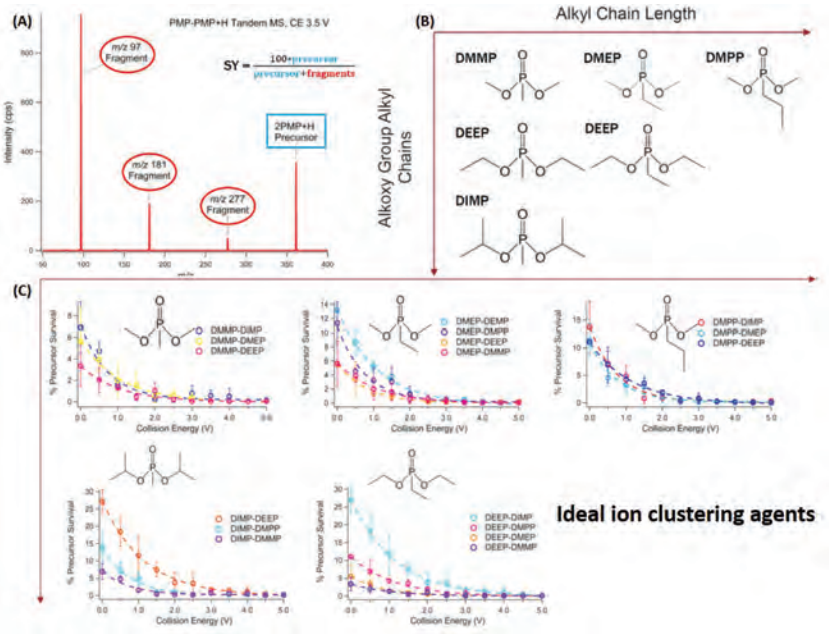


Figure 2: Experimental approach and results. Panel (A) shows the spectra used to calculate Survival Yield (SY) curves to determine proton affinities and potential clustering. Panel (B) shows the increasing clustering potential relative to functional group length and location. Panel (C) show the SY curves for a group of phosphate containing compounds.

Way Ahead

Dr. Clowers is now extending this technique to enable detection of halogenated compounds and is using his KRAFT technique as a method to separate molecular species. Collaborative efforts with Redstone Arsenal, Chemical Biological Center, Pacific Northwest National Laboratory, and Smiths Detection are ongoing. The Army can further capitalize on this discovery and develop this technique to be at the forefront of detection of trace levels of compounds commonly found in chemical warfare agents and other materials.

SUCCESS STORY

Urban Films as Active Environmental Interfaces

This research **revealed that environmental surface films are not uniform, and instead are heavily influenced by biological and other chemical factors.** These results are essential in predicting the fate and transport of persistent organic pollutants in soils and aqueous media.

This success supports these ARL Core Technical Competencies:

Protection Sciences

Computational Sciences

Challenge

Environmental surface films (urban films), formed via the aggregation and deposition of natural and anthropogenic atmospheric emissions onto solid surfaces, are capable of adsorbing large quantities of persistent organic pollutants (POPs), including volatile organic compounds (VOCs), polyaromatic hydrocarbons (PAHs) and polychlorinated byphenyls (PCBs). The organic pollutants that adsorb onto urban films can then be exchanged with soils, rivers, and groundwater through processes of (photo)chemical degradation, desorption, and deliquescence, significantly impacting human and

environmental health. The potential for urban films to act as a reservoir for POPs is hypothesized to depend on the morphology and maturation of the film itself as well as proximity to an emission source (Figure 3). Currently, the understanding of how these factors vary with geographic areas, speciation of film components, and exposure to a range of environmental parameters (e.g., ozone, UV photons, temperature) is lacking.

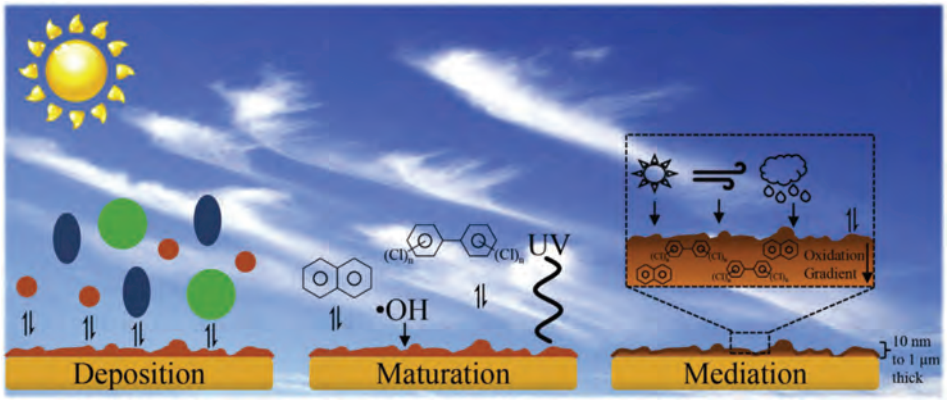


Figure 3: A schematic of the formation and maturation of environmental films. Deposition of particulare matter and small semi- or non- volatile species occurs continuously, but with seasonal and climatological variations. Maturation also occurs continuously, but will vary with geography and exposure. Mediation of fate and transport will depend on a suite of chemical parameters.

Action

In 2017, the ARO Environmental Chemistry program recognized an opportunity to investigate the complex dynamics of urban films, specifically aimed at determining the chemical characteristics that control POP uptake/release and how both the morphology of the surface film and adsorption of POPs is affected during film maturation. Because the literature surrounding urban films is still in its earliest stages of development, a number of investigative questions had to be explored to establish a framework for urban films: 1) How does the morphology of an urban film mature over its lifetime? 2) How do composition and morphology relate to POP uptake and release? 3) How is absorption of POP affected by the maturation of film components?

Dr. Scott Shaw, an Associate Professor at the University of Iowa specializing in the analytical chemistry of environmental interfaces, was uniquely qualified to explore the fundamentals of urban films through field-based sampling, experimental, and computational approaches. To answer the aforementioned questions, Dr. Shaw designed a synergistic research project where naturally occurring urban films were monitored in parallel with synthesized model film systems. By studying a combination of natural and experimental systems it would be possible to characterize the chemical interactions that control the behavior of urban films while also understanding which aspects of urban film chemistry dominated POP cycling over a range of spatial and temporal scales.

To determine how the morphology of an urban film matures over its lifetime a network of natural environmental films across an urban to rural gradient was established at the University of Iowa, allowing for frequent, passive sampling. The natural films were collected and subsequently characterized using chemical mapping techniques (e.g., POP composition, hydrophobicity, inorganic/organic molecule quantification) and morphology profiles (e.g., surface roughness, scanning electron microscopy). Spatially and temporally distinct samples were compared to determine if there were statistically significant differences as a function of distance to emission center or climate. One hypothesis at the outset of this research was that the dry season would serve as a sink for POPs onto urban films and the wet season would serve as a source of POPs to groundwater and soils.

This success was made possible by the following ARO S&Es or Program Specialists:

- Dr. Robert Mantz, ARO Chemical Sciences Division
- Dr. Elizabeth King, ARO Chemical Sciences Division

In parallel, model urban films were synthesized in the lab using mixtures of organic and inorganic (salt) species dispersed onto quartz substrates, a common building material in urban environments. The objective of this project was to create well-characterized films that accurately replicated the uptake and release behaviors of native films in order to determine which chemical characteristics disproportionately control adsorption/desorption dynamics. Once a suitable model film was developed, experiments were conducted to determine how these model films behaved under varying relative humidity (i.e., climate) in order to better predict the fate of film maturation and pollutant fate and transport.

The final objective of this project was to investigate the adsorption and desorption behaviors of (semi) volatile species in model and native films to quantify the amount of mass exchanged as well as the dynamics of exchange. These measurements will provide chemical level insight into the role of urban films in uptake and release of persistent organic pollutants and other species of interest.

Result

A number of surprising conclusions can be made from the results of the urban film studies. With respect to determining the maturation of urban films over time, samples collected from urban, suburban, and metropolitan locations were chemically characterized using time-of-flight (TOF) mass spectrometry (MS) and scanning electron and atomic force microscopy. Surface morphological features spanned six orders of magnitude (i.e., nm to mm scale) and were comprised of (semi) volatile molecules indicative of POPs. Furthermore, although films built rapidly within the first three months of growth showed there was a high degree of both temporal and spatial heterogeneity with particulate adsorption suggesting that film density appears to be indiscriminate on location and distance to emission center.

Results from the field sampling campaign also emphasized the importance of biological activity on urban films. Dr. Shaw used Fourier transformation ion cyclotron resonance secondary ion mass spectrometry and (FTICR-SIMS) and TOF-SIMS for chemical analyses and imaging of large molecular weight particulates found on urban films. Principle component analysis (PCA) of the organic and inorganic species enabled Dr. Shaw to fingerprint proteinaceous macromolecules consistent with fungal and bacterial microorganisms. This rich community of microorganisms may be a driving control for POP uptake and release on urban films that has been left out of previous models of transport. This work has fostered a number of collaborations efforts with the Pacific Northwest National Laboratory's (PNNL) Environmental Molecular Sciences Laboratory (EMSL) where the FTCIR-SIMS and TOF-SIMS used for chemical morphology mapping are operated by Dr. Chris Anderton and De. Zihua Zhu.

The results of model film portion of the study concluded that relative humidity is a dominant chemical parameter controlling the fate of urban films, and thus adsorbed POPs. Microscopy results indicate that deliquescence, the process by which a substrate absorbs moisture until it dissolves, does not scale with the organic and inorganic components of the model film (Figure 4). These results suggest that the behavior of urban films cannot be easily modeled with simple first-order reaction kinetics. Instead, additional research is required to understand the link between film type, maturation, transport and seasonality.

Results

- Co-authored publication between Pacific Northwest National Laboratory and academic researchers in the *ACS Earth and Space Chemistry* journal
- Collaboration between academic researchers and CCDC Chemical Biology Center to study the role of biology in the development and behavior of urban films.

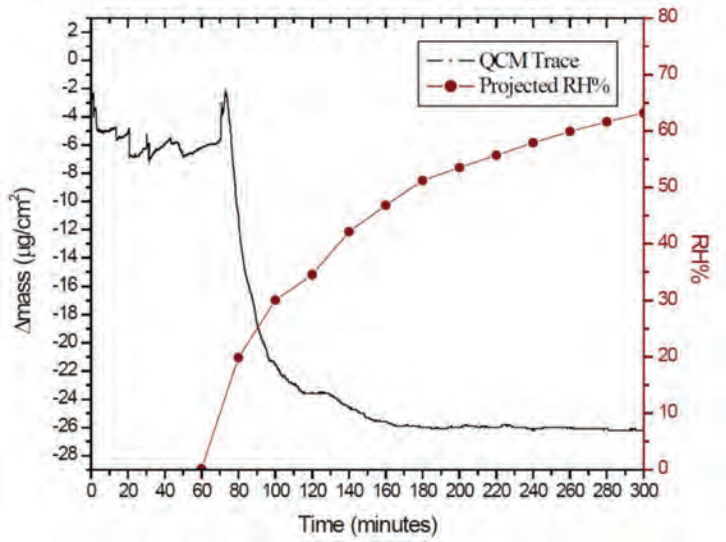


Figure 4: Apparent mass change recorded via quartz crystal microbalance (QCM) for a KNO3 film (solid black line) as a function of time as it is exposed to varying relative humidity (%RH; red line). The sharp decline in mass change at 60 minutes highlights the non-linear nature of deliquescence for urban films as a function of %RH.

Overall, these results have filled in a critical knowledge gap in environmental surface film science. Prior to this study, urban film models operated under the assumption that films are smooth and homogenous. However, these studies show that the topography of urban films varies by six orders of magnitude and is sensitive to film maturation and the biologic-organic-inorganic matrix from which the film is comprised.

Way Ahead

Dr. Shaw and his team are focusing their future efforts on experiments that will measure adsorptive and desorptive behaviors in model and native films. This project has led to several professional collaborations with staff scientists at PNNL-EMSL. Additionally, Dr. Shaw will be working in concert with researchers from the CCDC Chemical Biological Center to predict the fate and transport of volatiles and POPs in urban films, focusing on implications for remediation.

Molecular Structure and Dynamics Program

Current Scientific Objectives

01

Achieve control for state-to-state chemical reactions, quantum state preparation, and intermolecular interactions that if successful, will enable leap-ahead developments in Army materiel such as keyed detonation of explosives that are safer for transport, sensitive and selective chemical threat detection at range, and synthetic routes to new energetic materials

02

Model and explain novel dynamics phenomena, including reaction mechanisms and electron-transfer rates that if successful, will enable a deep understanding of chemical kinetics, thermochemistry, and catalysis for the design of new catalysts and energetic materials to manufacture compounds ranging from structural materials to explosives for the future Soldier

Program Manager

Dr. James Parker

Program Manager, Molecular and Structure Dynamics

Chemical Sciences Division

ARO Physical Sciences Directorate

Dr. Parker completed his undergraduate studies at Marquette University, receiving his B.S. in chemistry in 1993. He trained as a physical chemist at the University of Mississippi, receiving his Ph.D. in physical chemistry in 1999. He came to ARO in 2009 as the Program Manager for what was then called the Physical and Theoretical Chemistry Program.

SUCCESS STORY

Two-Electron Reduced Density Matrix Methods for Advanced Computational Chemistry

This ARO initiative resulted in the **development of new computational chemistry theories** which will enable scientists to synthesize next-generation materials for high-tech products in catalysis, solar energy conversion, explosives, and electronics.

This success supports these ARL Core Technical Competencies:

Materials and Manufacturing Sciences

Computational Sciences

Challenge

In 1995, the National Research Council ranked the development of two-electron reduced

This success was made possible by the following ARO S&Es or Program Specialists:

- Dr. James Parker, ARO Chemical Sciences Division

density matrix (2-RDM) methods as one of the top unsolved theoretical problems in chemical physics. 2-RDM theory is an alternative way of viewing electronic structure theory, and it promises polynomial scaling which makes it attractive to chemists and materials scientists who want to study systems where strong electron correlation is important. 2-RDM is the primary quantum variable in the method, as opposed to the many-electron wavefunction utilized in full configuration interaction (CI) or multi-configuration self-consistent field (MCSCF) methods. The challenge to realizing the new theory rested in solving what has been known as the N-representability problem, in other words, what are the necessary boundary conditions such that an N-electron system can be represented by a two-electron system.

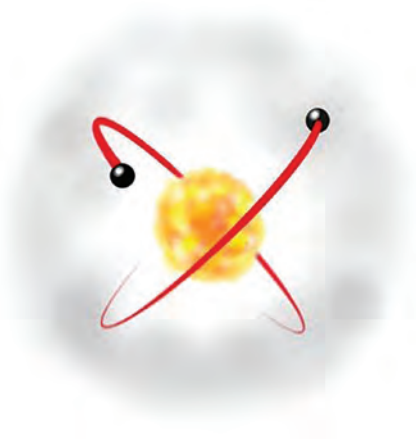


Figure 1: Figurative representation of an N-electron system by a 2-RDM (courtesy of University of Chicago).

The idea was originally posed by A. John Coleman (Queens University), Joseph Mayer (University of Chicago) and Per Olov Löwdin (University of Florida) in the 1950s. In the 1960s there was a series of international conferences that were organized to search for the N-representability conditions. Early confidence that researchers would work out these conditions quickly gave way to despair in the late 1960s. By then it appeared that there were potentially impossible barriers to the problem.

Action

In 2010 while on a site visit to the University of Chicago, Dr. James Parker recognized that the research ideas presented by Professor David Mazziotti presented a unique method to identify all of the necessary boundary conditions to satisfy N-representability. Professor Mazziotti's proposal was funded on 10 February 2011, and he made quick progress on the problem. In 2012, the journal *Physical Review Letters* published his paper, "Structure of Fermionic Density Matrices: Complete N-representability Conditions" in which all the boundary conditions for development of 2-RDM theory was contained. In the following years, Professor Mazziotti developed his own 2-RDM code to solve the electronic structure for many electron systems in which strong correlation was important, however his code had the limitation that it was not readily available to others.

Dr. Parker identified the high value of developing a commercial-quality 2-RDM code that could be used by the wider research community and DoD. These early discussions lead to a BAA in the STTR program and the formation of a new start-up company RDMChem in July 2014. Two STTR contract awards were made: one to University of Chicago/RDMChem (PI: Professor David Mazziotti) and one to Florida State University/Q-Chem (PI: Professor Eugene DePrince).

Result

Both projects made considerable progress toward the development of commercial products. Shortly after the end of the phase II STTR contract, Q-Chem released their first version of computational chemistry software built on reduced density matrices in August 2018. RDMChem released theirs on the MapleSoft platform in March 2019.

Results

- ARO funded research led to algorithms to predict chemical reactivity that are now available in two different products: MapleSoft and Q-Chem

Way Ahead

Researchers at ARL WMRD served as evaluators for the beta test version of the resulting commercial computer codes. They provided critical feedback on the operation of the code to the developers. The resulting code from both companies, released into MapleSoft and into Q-Chem, has strong advantages over the current state-of-the-art methods in ab initio quantum chemistry which rely on coupled clusters methodology. Two primary advantages of the 2-RDM code is that it offers increase in computational efficiency, especially with respect to scaling, while at the same time solving the electronic structure problem with only insignificant approximations taken. This is what makes the 2-RDM theory so promising: one can solve the electronic structure of an N-electron molecule with essentially no approximations, and therefore one has access to quantitative predictive power even for situations where strong electron correlation is present. Thus, in the future, it will become routine for chemists to build strong electron correlation into their models, so that design of future Army-critical technologies in catalysis, solar energy conversion, and energetic materials will become routine.

SUCCESS STORY

Synthesis of Amorphous Polynitrogen in Cold Liquid Plasma

This ARO initiative resulted in the **discovery of an all-nitrogen material** which may point the way toward making the next-generation disruptive energetic materials.

Challenge

Nitrogen, under extreme conditions, can form singly-bonded polymeric molecules. The breakdown of this singly-bonded material into nitrogen's diatomic state can result in an energy release among the largest for any chemical reaction, making the material potentially ideal for explosives and propellant applications. Following theoretical predictions, several forms of polymeric nitrogen were discovered and synthesized either as a crystalline material or as a disordered network of singly-bonded nitrogen atoms. Until now, extremely high pressures (tens of gigapascals) have been needed to synthesize all-nitrogen polymers, and this has prevented their practical application. Additionally, the polymeric materials created at ultra-high pressures are not stable when brought to ambient conditions, further hindering their utility.

Action

In 2017, the Chemical Sciences Division set up a new thrust area in synthesis of novel, disruptive energetic materials. Dr. Robert Mantz was the acting program manager at this time. During conversations with Dr. Jennifer Ciezak-Jenkins (ARL WMRD) the two of them identified Professor Danil Dobrynin of Drexel University as a potential PI for the program. Professor Dobrynin was known for his work in liquid plasmas, and he was asked to submit a proposal to study the effect of high voltage pulsed discharge in liquid nitrogen. The proposal was officially awarded a grant on 01 November 2017.

This success supports these ARL Core Technical Competencies:

Ballistics Sciences

Materials and Manufacturing Sciences

This success was made possible by the following ARO S&Es or Program Specialists:

- Dr. James Parker, ARO Chemical Sciences Division
- Dr. Robert Mantz, ARO Chemical Sciences Division

Results

- Formation of a novel energetic material has been observed upon electrical discharge in liquid nitrogen.
- Characterization and stabilization experiments are ongoing to determine the nature of the material and whether it can be used in Army applications.

Result

Late in 2017, at the decision of the Directorate Director of Physical Sciences, management of the disruptive energetic materials thrust area was transferred to Dr. James Parker. Dr. Parker made a site visit to Drexel University in February 2018 to meet with Professor Dobrynin and to get a first-hand look at the experiments. Professor Dobrynin and his students demonstrated the experimental electric discharge apparatus for ARO representatives, with the result of producing a dark material which condensed in the bottom of the flask containing the liquid nitrogen. At the time, they were not able to say what the material was since they were lacking analytical methods, however they hypothesized that it could be polynitrogen. Upon evaporation of the liquid nitrogen and warming, the material reacts violently producing sound and light. Professor Dobrynin postulated that the material is a solid, amorphous non-molecular form of nitrogen. Dr. Parker wanted to be sure of this and so he encouraged Professor Dobrynin to undertake analytical experiments right away. Analysis by Raman spectroscopy showed that no ozone or azide had formed in the material, and the spectroscopy hinted at the presence of N-N single bonds. After allowing the sample to warm and react in the presence of air, analysis of the reaction products by infrared spectroscopy was undertaken. Results of infrared spectroscopy show that N_2O and ozone are products of the sample's reaction in air. In order for these products to form, it is hypothesized that the following reactions involving excited diatomic nitrogen, $N_2(A)$, occur:

$$N_2(A) + O_2 \rightarrow N_2(X) + O + O$$

$$O + O_2 + M \rightarrow O_3 + M$$

$$N_2(A) + O \rightarrow N_2O + O$$

The observed formation of both O_3 and N_2O products can be explained by significant energy release during the sample decomposition. Due to the absence of NO and other similar species, Professor Dobrynin hypothesizes that one possible mechanism of such rapid production of both nitrous oxide and ozone during the sample decomposition is related to energy release and production of excited nitrogen in the above reactions. This is somewhat surprising since production of electronically excited nitrogen $N_2(A)$ requires energies on the order of 6.2 eV and it is not typically produced during explosions. On the other hand, the N ≡ N triple bond energy is characterized by the value of 9.9 eV, while the N = N double and N–N single bond energies are 4.3 eV and 1.6 eV respectively. Back conversion to diatomic molecular nitrogen is, therefore, highly exothermic and the corresponding energy release could be the source of production of electronically excited nitrogen, which leads to generation of N2O. Professor Dobrynin is not definitively claiming production of polynitrogen material in the experiments, but multiple N_x all-nitrogen compounds could be formed in the non-thermal plasma in liquid nitrogen.

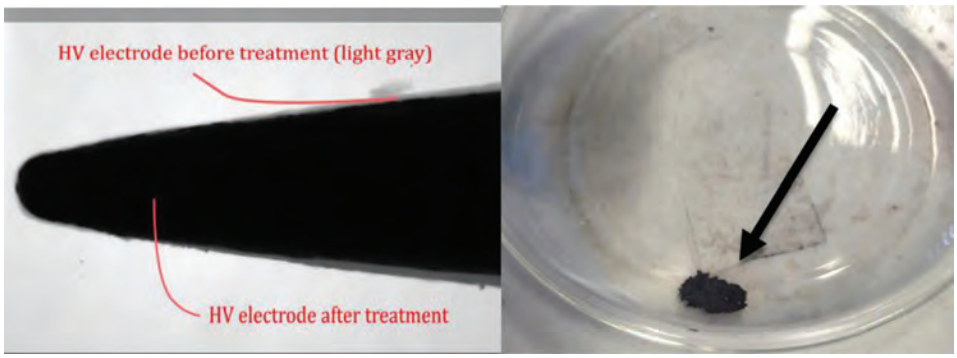


Figure 2: Black powder material produced after one hour pulsed plasma treatment and evaporation of excess liquid nitrogen.

Way Ahead

In future years, Professor Dobrynin will establish collaborative studies with Dr. Jennifer Ciezak-Jenkins of CCDC ARL WMRD in order to definitively characterize the material. These researchers plan to set up an x-ray diffractometer which will allow elucidation of the molecular structure. If confirmed to be polynitrogen, this would be the first time that the substance would have been produced in macroscopic amounts at one atmosphere pressure. They also have plans to stabilize the material using activated carbon and/or porous ceramic. Professor Dobrynin has filed for a patent on synthesis of novel materials using kHz pulsed discharge in liquid nitrogen.

Polymer Chemistry Program

Current Scientific Objectives

01

Develop new approaches for synthesizing polymers with precisely-defined microstructure and composition that if successful, will provide the first-ever methods for the design and synthesis of polymers with precise control of molecular structure, thereby enabling new capabilities for Army materiel, ranging from protective coatings to targeted therapeutics

02

Devise strategies to control polymer assembly and responsive behavior at the molecular level, that if successful, will render complex materials with programmed and precisely-defined functions such as self-sensing or self-repairing materials

Program Manager

Dr. Dawanne Poree

Program Manager, Polymer Chemistry
Program Manager (Acting), Reactive Chemical Systems
Chemical Sciences Division
ARO Physical Sciences Directorate

Dr. Poree completed her undergraduate studies at Nicholls State University, receiving her B.S. in Chemistry in 2004. She trained as a polymer chemist at Tulane University, receiving her Ph.D. in Chemistry in 2010. She came to ARO in 2011 as a SETA Contractor to support the Polymer Chemistry Program, and was hired as the Program Manager in 2014. In addition, Dr. Poree has served as the Acting Program Manager for Reactive Chemical Systems since 2014.

SUCCESS STORY

Research Integrating Chemistry and Synthetic Biology Led to New BioBit™ Educational Platform

This ARO initiative led to the unexpected result of an **educational platform to train the next generation of scientists** in synthetic biology.

This success supports these ARL Core Technical Competencies:

Materials and Manufacturing Sciences

This success was made possible by the following ARO S&Es or Program Specialists:

- Dr. Dawanne Poree, ARO Chemical Sciences Division
- Dr. Stephanie McElhinny, ARO Life Sciences Division

Challenge

The method and field of synthetic biology aims to program biological systems to carry out useful functions. This field has made meaningful progress toward the biomanufacturing of medicines, sustainable chemicals, and advanced fuels, as well as cellular diagnostics and therapies. At the core of these advances is the ability to control and tune the processes of transcription and translation, potentially offering access to non-natural materials that cannot be made by any other means. As an example, the translation apparatus is the biological cell's factory for protein synthesis. The ribosome is a molecular machine that polymerizes α-amino acids into proteins through the creation of amide bonds. It is the catalytic workhorse of the translation apparatus, with protein synthesis rates of up to 20 amino acids per second at an accuracy of 99.99%. The extraordinary catalytic capacity of the translation machinery has attracted extensive efforts to engineer it to generate other polymers beyond natural proteins.

Most research efforts in this area have focused on the site-specific incorporation of unnatural α-amino acids into proteins by the natural translation apparatus; however, the potential to engineer the ribosome to perform alternative chemistries beyond the amide bond formation remained virtually unexplored.

Action

In 2015, recognizing emerging advances in synthetic biology, and particularly the development of in vitro systems capable of modifying biological translation machinery, Drs. Poree and McElhinny conceived of a MURI topic focused on re-engineering the translation machinery to accept and polymerize non-biological monomers in a sequence-defined manner. Sequence defined polymers (SDPs) are linear macromolecules whose chemical and physical properties can be programmed with atomic-scale resolution. It has been impossible, so far, to produce finely tailored non-natural SDPs (i.e., materials of defined atomic sequence, exact monodisperse length, and programmed stereochemistry), yet the development of synthetic routes toward these molecules promises technological breakthroughs in advanced functional materials, nanotechnology, electronics, and beyond. To achieve this ambitious goal, the MURI team, led by Professor Michael Jewett of Northwestern University, proposed to develop novel cell-free biosynthetic platforms that enable the generation and evaluation of modified ribosomes and other translation factors in a non-cellular, in vitro setting. This dramatically expands the ribosome design space accessible to the team, as ribosomes are essential for cell viability and only limited ribosome mutations are possible in cells. While the team has made several notable advances in the development of a

cell-free ribosome construction platform as well as analytical tools for single molecule characterization of SDPs, this work has made possible the serendipitous development of a modular synthetic biology educational kit that can greatly enhance the teaching of science, technology, engineering, and math (STEM) concepts while also making cutting-edge science easy to use and accessible.

Result

The MURI team demonstrated that the cell-free systems developed as part of the MURI effort can be freeze-dried along with genetic elements to form pellets that are stable at room temperature and easily transported between team members. The shelf-stable nature of these freeze-dried, cell-free (FD-CF) pellets eliminates the need for dedicated refrigerators or freezers. In addition, FD-CF reactions do not require any specialized equipment, making them a robust technology for using synthetic biology in low-resource environments. While, from an Army perspective, this makes these systems ideal for enabling on-demand chemical production in remote environments, the unique practicality of the FD-CF technology also renders them highly suitable for applications in biology education where there is currently a glaring lack of hands-on synthetic biology experiments. To explore the FD-CF technology as an educational tool, the research team partnered with Chicago-area teachers to develop curricula for high school math and middle school science classes, to emphasize the cross-cutting nature and the value of this activity at various educational levels. The resultant BioBitTM Explorer and BioBitTM Bright kits included a set of demonstrations designed to engage three of the five senses – sight, smell, and touch – through the expression of proteins in FD-CF reactions that produce fluorescence, enzyme-generated fragrances, and large-scale hydrogels, respectively (Figure 1).

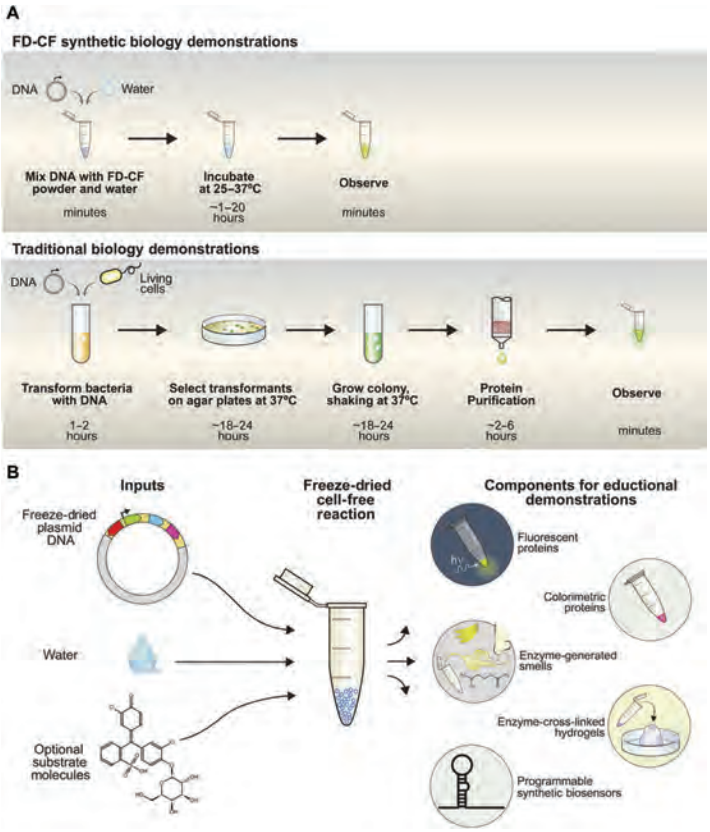


Figure 1: BioBit™ educational kits based upon FD-CF technology

Results

- Two Science Advances publications on the BioBits™ Bright and Explorer platforms
- BioBits™ Bright and Explorer kits commercialized by miniPCR bio™, now available to educators
- BioBits Bright™ has been used by ARL SEDD as part of an Army-sponsored STEM outreach program

Figure 2: BioBit™ kit designed to be used by students and teachers with no biological training. Kits are also designed to be modular to allow students/teachers to design their own experiments.

These outputs provide demonstrations that can be used to teach fundamental biology concepts and principles of tunable protein expression, enzyme catalysis, and material properties. An additional module was also created that allows students to take DNA extracted from fruit and analyze the samples using toehold switch sensors designed to detect specific DNA sequences from the banana and kiwi genome, allowing for the first-ever student experiments that enable probing of DNA on the genetic level (Figure 2). Notably, the toolkits are designed to be modular, allowing teachers to tailor the demonstrations to their curricula. Because of the highly portable, cost-effective, and user-friendly nature of the reagents and laboratory activities, the BioBits™ Bright and Explorer kits have utility both inside and outside of a formal classroom or laboratory setting. Thus, these resources promise to increase access to cell-free technologies, enhance basic biology education, and increase participation in the field of synthetic biology which will be essential for realizing scientific discoveries in the 21st century.

Way Ahead

For the Army, research in synthetic biology will be essential for realizing scientific discoveries necessary to render next-generation advances in responsive materials, game-changing chemical, material, and drug manufacturing methods, the detection and elimination of toxic chemicals, and medical applications ranging from the detection and treatment of traumatic brain injury to the development of integrated prosthetics. If the United States is to maintain leadership in the field of synthetic biology in the coming decades, current elementary, middle school and high school students must be encouraged to pursue long term study in this field. The BioBits™ kits provide an ideal platform for teaching advanced molecular and synthetic biology concepts in a hands-on manner. The research team has already partnered with ARL SEDD to provide BioBits Bright™ as part of an Army-sponsored STEM outreach program. Beyond the educational platform, the MURI team is continuing to extend the boundaries of cell-free synthetic biology to enable re-engineering of the ribosome's active site to promote novel non-natural polymer synthesis.

SUCCESS STORY

Novel Method for Achieving Controlled Polymer Stereochemistry for Emergent Material Properties

This ARO initiative resulted in the **discovery of catalysts capable of synthesizing a type of polymer with precise control of its molecular geometry**, providing ten-fold stronger adhesion of the polymer without the use of an adhesive.

This success supports these ARL Core Technical Competencies:

Materials and Manufacturing Sciences

This success was made possible by the following ARO S&Es or Program Specialists:

- Dr. Dawanne Poree, ARO Chemical Sciences Division

Challenge

Control of polymer stereochemistry is well known to improve the properties of otherwise chemically identical atactic materials (i.e., materials composed of identical chemical formulae but that differ in the 3D orientation of their atoms). This is perhaps best exemplified by polypropylene in which racemic polypropylene is an amorphous viscous liquid, but access to isotactic and/or syndiotactic polypropylene provides a low density, commodity thermoplastic used in everything from packaging material to textiles to medical devices. Unfortunately, well-developed stereoselective polymerization methods currently only exist for specific types of polymers (non-polar olefins such as propylene). Controlled polymerization techniques developed of the past three decades provide excellent control over polymer length and chain-end functionality; however, there are no effective methods for controlling the chain-end stereochemical environment in these ionic- and/or radical-based polymerization mechanisms.

Action

In 2018, inspired by the power of tacticity to act as controlled, tunable handle for the tailoring of bulk polymer properties, the ARL ARO Polymer Chemistry Program Manager Dr. Dawanne Poree began focusing programmatic resources on the development of novel catalysts and synthetic techniques that enable polymerization of functional monomers with stereochemical control. Of particular interest was using tacticity control to enable multifunctional materials that combined novel engineering properties (mechanical and thermal stability) with other beneficial, Army-relevant functions. As one approach to achieving this goal, Dr. Poree strategically supported researchers at the University of North Carolina - Chapel Hill (UNC-CH) to design novel catalysts for the stereoselective polymerization of vinyl ether monomers to render stereo-controlled polar polyolefins with the vision that these materials would possess the same thermoplastic behavior as their non-polar counterparts, but with “built-in” functionality that allows them to be interfaced with other materials, thus extending their utility beyond packaging materials, and into next-generation composites, adhesives, and electronics. Unfortunately, achieving stereo-control over polar olefins is non-trivial. The primary means of controlling polymer stereochemistry is through coordination-insertion polymerization which uses a transition metal catalyst to regulate the facial addition of each monomer which enables a highly stereoselective polymerization. A fundamental limitation to coordination-insertion polymerization, however, is that these early transition

Results

- Discovery of a new class of stereoselective polymerization technique that enables the synthesis of polyvinyl ethers with precise control of their molecular geometry, providing ten-fold stronger inherent adhesion in a plastic
- Publication in *Science*
- Presented invited seminar at CCDC ARL WMRD

metal catalysts bind to polar groups irreversibly, resulting in no polymerization. While other means of polymerizing polar olefins do exist, the resultant poly (vinyl ethers) (PVEs) have virtually no stereo-control and poor mechanical properties. To address this 60+ year old challenge, the UNC-CH research team, led by Professor Frank Leibfarth, sought to develop a novel catalytic approach to systematically bias the reactivity and chain-end stereochemical environment during a cationic polymerization.

Result

More specifically, the research team's approach employed chiral anion catalysis which had previously been used to control the stereochemistry of small molecules. They hypothesized that because cationic polymerization takes place in a solvent with a low dielectric constant, the cation at the propagating, or growing, end of the polymer chain would tightly pair with the chiral anion of the catalyst which would dictate which side of the chain the next monomer will add to, resulting in the formation of polymers with high structural regularity (Figure 3). Using this catalytic method, the research team was able to polymerize a variety of vinyl ethers with isotacticity, demonstrating 88-93% stereoselectivity depending on the monomer substituent (Figure 4). For each of these substituents, this is the highest stereoselectivity reported in the literature. Also notable is the immediately apparent influence of stereochemistry on the materials properties. While traditional polymerization methods give the amorphous PVEs shown on the left, chiral counterion-based catalyst developed in this effort renders semicrystalline thermoplastics, shown on the right, with melting points between 70-140°C.
These two materials are chemically identical, and are simply just stereoisomers of each other, demonstrating how controlled stereochemistry can lead to emergent material properties.

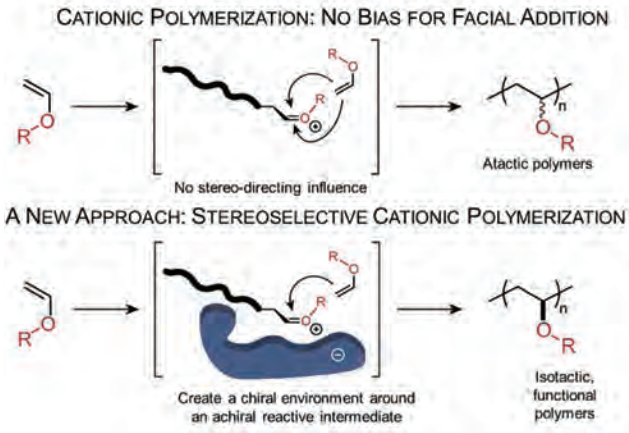


Figure 3: Design of a stereoselective cationic polymerization

In exploring the mechanical properties of the isotactic PVEs, the materials were shown to possess tensile properties comparable to those of commercial low-density polyethylene, but with more than an order of magnitude stronger adhesion (Figure 5), indicating their promise for next-generation engineering applications. These findings, coupled with the scalability of the polymerization procedure (multi-gram polymerizations achieved), the high processability of the resulting material (which can be melted, molded, and cooled), and the broad monomer scope signify an important breakthrough in the polymer field.

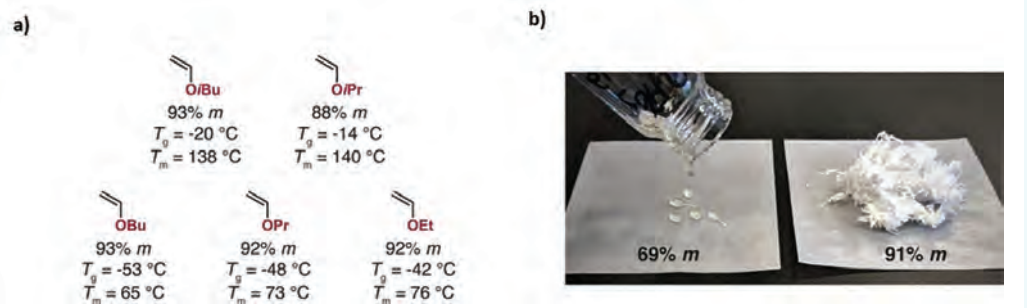


Figure 4: a) Monomer scope demonstrating generality of the stereoselective polymerization methodology; b) visual representation PVEs prepared via traditional methods (left) and the new stereoselective method (right).

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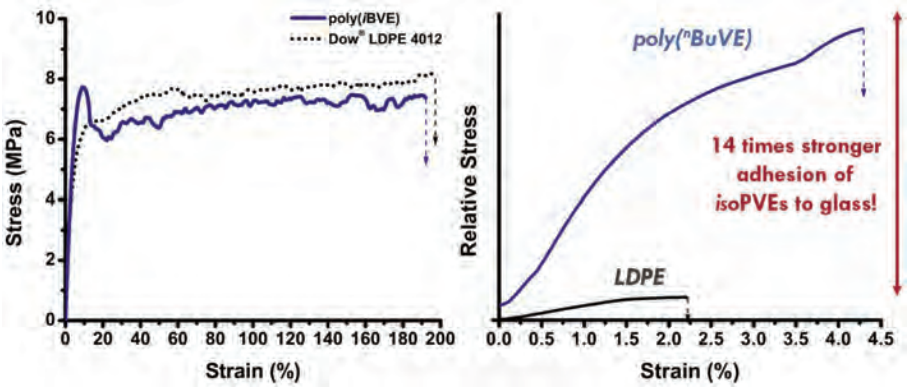


Figure 5: Mechanical and Adhesive properties of isotatic poly (isobutyl vinyl ether) in comparison to commercial low-density polyethylene

Way Ahead

This research represents an important step towards introducing stereo-control in polymerizations beyond just hydrocarbon-containing monomers. Future work will focus on translating this concept to other polymerization systems as this could rapidly push polymer manufacturing toward more highly functional materials, potentially rendering plastics that can bind tightly to glass, metal, or tissue that will provide protective coatings for equipment, biomedical devices to treat the Soldier, or adhesives for less expensive and lighter structural materials. Transition opportunities are currently being explored with the ARL Science of Manufacturing at the Point of Need Essential Research Program. ARL hosted Professor Leibfarth on a visit to discuss mutual interests in light weight thermoplastics with enhanced adhesive properties. Collaborative efforts among CCDC ARL ARO and WMRD and potentially CCDC SC will be further sought and leveraged to transition key knowledge products towards the development of new protection capabilities for the Soldier.

Reactive Chemical Systems Program

Current Scientific Objectives

01

Create chemically and biologically functionalized surfaces with precise control of structure and function that if successful, will lead to novel decontaminants, sensors, and coatings for Soldier protection

02

Attain a mechanistic understanding of mass transport, adsorption, and reactivity on surfaces and at interfaces that if successful, will lead to novel materials and catalysts for degrading chemical threats to protect the Soldier

03

Design and synthesize chemical systems that sense and respond to external stimuli that if successful, will lead to intelligent materials for Soldier protection

Program Manager

Dr. Dawanne Poree

Program Manager, Polymer Chemistry

Program Manager (Acting), Reactive Chemical Systems

Chemical Sciences Division

ARO Physical Sciences Directorate

Dr. Poree completed her undergraduate studies at Nicholls State University, receiving her B.S. in Chemistry in 2004. She trained as a polymer chemist at Tulane University, receiving her Ph.D. in Polymer Chemistry in 2010. She came to ARO in 2011 as a SETA Contractor to support the Polymer Chemistry Program, and was hired as the Program Manager in 2014. In addition, Dr. Poree has served as the Program Manager (A) for Reactive Chemical Systems since 2014.

SUCCESS STORY

Increasing Catalytic Efficiency with Single Atom Catalysts

This ARO initiative resulted in demonstration of a **single atom catalyst with an efficiency rate 25 times higher than its traditional nanoparticle catalyst counterpart,** and identification of the structure of the isolated atoms during a simple probe reaction.

This success supports these ARL Core Technical Competencies:

Protection Sciences

Materials and Manufacturing Sciences

Challenge

Supported metal nanostructure catalysts are critical for a variety of applications including environmental remediation, energy platforms, and pharmaceutical development. Despite their wide employment, supported metal catalysts are typically comprised of a mixture of nanoparticles and sub-nanometer clusters, and this heterogeneity can reduce catalytic efficiency, trigger undesired side reactions, and make identification of the active site problematic. Recently, there has been significant interest in single-atom catalysts (SACs) where isolated metal atoms are singly dispersed on supports, maximizing atom utilization efficiency and offering unique electronic properties. While literature has shown individual studies of metal-supported catalysts, there are minimal reports of a systematic study comparing both metal nuclearity (nanoparticle, sub-nanometer cluster, or single atom) and support and their impact on both catalytic activity and selectivity.

Action

To address one of the program's objectives of understanding reactivity on nanostructured surfaces, previous ARL ARO Program Manager, Dr. Jennifer Becker, strategically supported research in metal oxide nanoparticle catalysts. These investments encompassed synthetic methods towards nanostructured catalysts with well-defined morphologies and properties as well as novel spectroscopic tools, such as ultra-high vacuum techniques, for subsequent surface analysis. In order to advance reactive and selective catalytic materials beyond traditional metal oxides, Dr. Poree identified SACs as a potential new focal area and initiated a Single Investigator project with Professor Ayman Karim at Virginia Polytechnic Institute and State University to begin differentiating the mechanisms and catalytic properties of metal atoms and small clusters.

Result

In FY19, the Virginia Tech research team discovered that single-atom versus traditional nanoparticle Ir-on-MgAl2O4 catalysts demonstrate a 25 times higher catalytic efficiency rate for low temperature CO oxidation. Using a combination of detailed kinetic studies, state-of-the-art in situ/operando spectroscopic tools, and quantum chemical calculations, the research team provided a very detailed atomic level insight into the structure and reaction mechanism of iridium single-atom catalysts for the probe reaction.

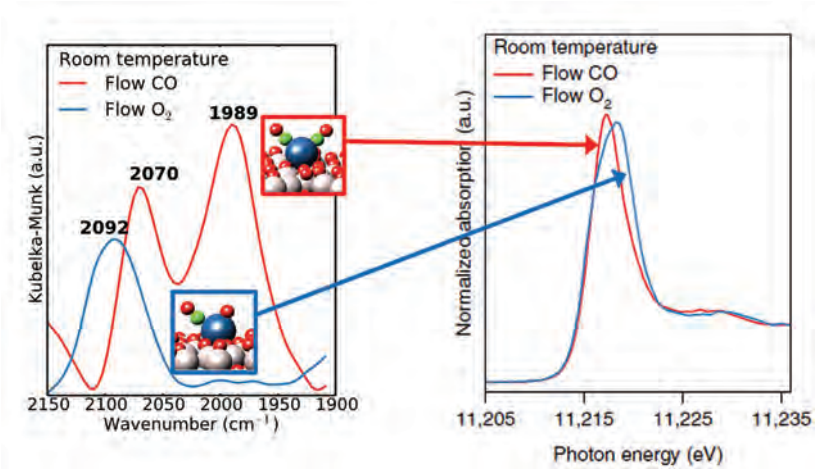


Figure 1: In situ infrared spectroscopy (left) and HERFD-XANES (right) of CO adsorbed on 0.0025% Ir/MgAl2O4 at 25°C.

This success was made possible by the following ARO S&Es or Program Specialists:

- Dr. Dawanne Poree, ARO Chemical Sciences Division

Results

- First proven mechanism for CO oxidation on supported single atom catalysts
- Demonstrated and differentiated single atom and sub-nanometer cluster activity with Ir-based complexes
- Research results transitioned to a new FY20 joint DTRA-CCDC-Chemical Biological Center program on "an every-atom-counts" approach to designing small cluster catalysts

The oxidation kinetics for CO for single atoms and nanoparticles revealed different reaction orders. The CO and O2 orders were -1 and +1 on the nanoparticle, as typically observed on large metal nanoparticles supported on non-reducible oxides. However, the CO and O2 orders were approximately +1 and 0 on single Ir atoms, indicating that the reaction mechanism is significantly different for single atoms. To provide insight on the reaction mechanism, and specifically the O2 activation step on Ir single atoms, the research team performed in situ diffuse reflectance infrared Fourier transform spectroscopy (DRIFTS) and high-energy-resolution fluorescence-detected (HERFD) X-ray absorption near edge spectroscopy (XANES) experiments of adsorbed CO, followed by exposure to O2. Similar changes were observed in both spectra for partial oxidation of the Ir metal and were consistent with DFT calculations. Operando HERFD-XANES measurements uncovered critical features of the CO oxidation mechanism: the Ir(CO)(O) is the most stable intermediate (resting state of the catalyst); Ir(CO) is the active supported complex; and CO oxidation on Ir single atoms proceeds via an Eley-Rideal mechanism, consistent with the +1 and 0 orders identified in the kinetic studies. The results highlight the importance of combining in situ/operando spectroscopy, together with quantum chemical calculations and kinetic measurements to attain a complete picture of supported single atom catalysis. These results were reported in Nature Catalysis.

Way Ahead

Understanding atomic level mechanistic details of supported single atom catalysts will lay the foundation towards designing novel catalysts with superior activity and selectivity for the detection and destruction of toxic industrial chemicals and chemical threats. While the research has noted differences in mechanism and ultimately activity between single atoms and nanoparticles, studies have been limited to a single model catalyst. With additional support from ARO (Dr. Dawanne Poree), Virginia Tech researchers will expand the metal identity and metal support, and begin to identify descriptors for predicting activity of supported single atom catalysts for more complex reactions. Collaborative efforts among CCDC ARL ARO, WMRD, CCDC-CBC, and DTRA will be sought and leveraged to transition key knowledge products towards the advancement of new protection capabilities for the Soldier.

SUCCESS STORY

Rapid Detection and Identification of Biological Events

This joint ARO-Joint Science and Technology Office for Chemical and Biological Defense (JSTO-CBD) SBIR/STTR Program initiative resulted in **fast detection of biological simulants with excellent sensitivity.**

This success supports these ARL Core Technical Competencies:

Protection Sciences

Materials and Manufacturing Sciences

Challenge

Protection of infrastructure from biological threats requires the ability to rapidly identify aerosolized materials that can include a wide range of biological components including spores, vegetative bacteria, viruses, and toxins. Beyond the biological threat, low vapor pressure chemical threats could be attached to particulate and dispersed as an aerosol.

Furthermore, the availability of gene editing tools such as CRISPR/Cas9 increases the possibility of engineered agents designed to avoid detection. Addressing this broad range of threats requires the ability to move beyond the limitations posed by currently deployed biological detection systems which typically require threat specific assays to recognize a specific molecular target.

Action

To address the military's need for rapid, accurate, sensitive, and low cost per test detection of biological agents, CCDC ARL ARO Program Manager, Dr. Poree, in collaboration with the Joint Science and Technology Office for Chemical and Biological Defense (CBD) Small Business Innovation Research (SBIR) and Small Business Technology Transfer (STTR) Programs, Mr. Larry Pollack, oversaw the development and maturation of a novel mass spectrometry-based detection platform (SBIR Topic CBD14-101). The detection system combines advanced mass spectrometry and sample processing techniques with state-of-the-art microfluidic tools for a field robust detection capability that is anticipated to be significantly faster than current detection platforms.

Result

Zeteo Tech Inc. was awarded sequential Phase II funding (FY17) from the CBD SBIR Program to advance a Matrix-Assisted Laser Desorption and Ionization (MALDI) Time-of-Flight (TOF) Mass Spectrometry (MS) platform coupled with a trigger sensor for threat recognition. This approach was pioneered by the firm's academic partner at the Johns Hopkins University Applied Physics Lab in the late 1990's and subsequently adopted commercially for clinical diagnostics through the efforts of Bruker (with Becton Dickinson) and Shimadzu (with bioMérieux). Analytical systems developed by these companies have become gold standard assays in the clinical diagnostics industry. This top-down approach is used for rapid, presumptive identification of aerosolized biologicals.

In FY19, Zeteo Tech completed the design and build of an alpha version of the Zeteo Threat Agent Detection System (ZTADS), currently trademarked under BioFlyte™ 100. The prototype instrument automates all functions including sample acquisition and preparation and data acquisition and processing to extract critical features and identify threats.

Figure 2: Zeteo BioFlyte™ 100

Way Ahead

With additional funds from the CBD SBIR/STTR Program and Phase III customer funding, Zeteo Tech will continue to optimize the BioFlyte™ 100 platform to improve system features. Continued collaborative efforts among ARO, the JSTO-CBD SBIR/STTR Programs, and government customers will be sought and leveraged to develop and transition new detection and protection capabilities to the DoD.

This success was made possible by the following ARO S&Es or Program Specialists:

- Dr. Dawanne Poree, ARO Chemical Sciences Division

Results

- Demonstrated excellent detection sensitivities with biological simulants
- Awarded Phase III funding in FY19 to complete a prototype for further assessment

Behavioral Sciences Program

Physical Sciences Directorate

- Chemical Sciences Division
- **Life Sciences Division**
- Physics Division
- UARCs Division

Current Scientific Objectives

01

Identify and validate measurement methods to detect shifts in human behavior and collective action that if successful will lead to new tools to identify emergent conflict, violent extremist individuals and groups, and deception attempts by adversaries

02

Generate and validate predictive approaches to causally model emergent risks across individual, collective, organizational, and state levels that if successful will provide decision-makers with improved operational effectiveness for early identification of emergent security risks at these different levels

03

Investigate interdependencies among social, natural, and physical systems to determine the spatial and temporal evolution of dynamics that if successful will enable long-range prediction of precursors of conflict and enable early prevention and mitigation strategies

Program Manager

Dr. Lisa Troyer
Program Manager, Behavioral Sciences
Life Sciences Division
ARO Physical Sciences Directorate

Dr. Troyer completed her undergraduate studies at the University of Washington, receiving her B.A. in Sociology in 1989. She trained at Stanford University, receiving her Ph.D. in Sociology in 1995. She came to the Army Research Office in 2013 as a Scientific and Engineering and Technical Assistant to support development of programming in the behavioral sciences. In 2015, she was appointed as Program Manager of the Behavioral Sciences Program, Life Sciences Division.

SUCCESS STORY

New Computational Models for Predicting Adversarial Collective Action

This ARO initiative resulted in **new models to improve ability to predict how collective action unfolds in adversarial, allied, and neutral social groups** that will lead to the ability to scan and predict nefarious and friendly group action in the multi-domain operational environment.

Challenge

In the social sciences, collective action is not simply an additive function of the behaviors of individuals who comprise the collective. Group outcomes are the result of complex relationships among actors, compounded by individual differences in how those relationships are perceived and navigated. Moreover, groups do not function in isolation. They are embedded in networks of other groups – neutral, adversarial, allied – and the relationships among groups are a constantly changing dynamic. To further complicate the problem complete data on collectives is lacking. Often membership in real-world groups is only partly known and data on the attributes of even known members may be missing. Consequently, reliably modeling collective action to facilitate development and testing of predictive theories of social dynamics is a critical hurdle to overcome. Traditional methods relying on additively combining states and traits of individual actors (often self-reported) to predict collective action are neither reliable nor accurate when it comes to quantifying social dynamics. Such approaches suffer from large unexplained variance and low power making them poor candidates on which to base strategic decisions. Also, they tend to rely on continuous linear models that assume independent observations; but social dynamics often depart from continuous evolution and violate assumptions of independence. Thus new methods are needed model collective action.

Action

In FY15, Dr. Troyer began developing a new thrust in the Behavioral Sciences Program to address biases in traditional approaches to modeling collective action. Dr. Troyer has over two decades of research on social dynamics in collectives that impact decision-making outcomes. Collectives are characterized by a number of dynamics that affect collective action. Some entail process losses such as groupthink (characterized, in part, by false perceptions of the out-group as weak and morally corrupt), polarization effects (in which a group tends to make decisions that are more extreme than those of individuals), Ringlemann effects (describing exponential decrements in performance as group size increases), and evaluation apprehension (when individuals limit contributions to the group for fear of censure and the negative repercussions that follow). Moreover, these effects are exacerbated as problems become increasingly uncertain, size of the collective increases, and riskiness of the decision is amplified. Key phenomena that process losses affect are (1) shifts over time in collective outcomes in relation to collective resources; (2) the tendency of different groups to form and dissolve coalitions. Yet, results describing when these losses impact collectives and how they combine are inconsistent. Traditional work on these phenomena have focused on economic models of contributions to public goods. These approaches, however, fall short because they involve assumptions that artificially constrain choice (e.g., only binary choices are modeled, perfect rationality is assumed, group members have full knowledge of the resources and behaviors of all group members); continuous linear relationships between group composition and outcomes are assumed; and egalitarian resource distributions are set as initial conditions. These assumptions, however are often violated in real social encounters. To exacerbate the analytic difficulties of modeling social phenomena, data are often sparse and exclude data from high impact actors. Dr. Troyer has developed an innovative strategy to address these existing challenges for modeling social dynamics.

Following participation in two workshops in FY15 – one at Carnegie Mellon University on complex geosocial systems, and one at Harvard University on emerging models for

This success supports these ARL Core Technical Competencies:

Human Sciences

Network and Information Sciences

Computational Sciences

This success was made possible by the following ARO S&Es or Program Specialists:

- Dr. Lisa Troyer, Life Sciences Division

social dynamics – Dr. Troyer began receiving white papers that described potential projects to test established social theories using new modeling approaches commonly found in life and physical sciences that could overcome the biases that often plagued traditional approaches in the social sciences. These approaches have the potential to overcome deficiencies in modeling social dynamics and enable analyses of how large-scale collective action evolves.

The scientific impact of energizing a program to systematically address these issues is already being demonstrated. Dr. Troyer selected work by Dr. Sergey Gavrilets at the University of Tennessee – Knoxville who had previously developed mathematical models based on evolutionary biology to examine conflict and cooperation in non-human social groups (e.g., chimpanzees, spider monkeys, hyenas). Building on this work, he proposed a strategy for modeling large-scale human collective action that combines insights from economics public goods contests (in which groups and individuals compete for resources), with five important twists: First, he introduces a non-linear function to the models focusing on both focal and competing groups. Second, the model enables the ability of individuals to vary strategies continuously. Third, the difference in individual resources within the group are incorporated into the model, but full information among all actors is not required. Fourth, the project would validate the model (which had been built for non-human social groups, but not validated) in human social collectives. Fifth he incorporates the concept of dysphoric (threatening, painful) experience vs. euphoric (successful, enjoyable) events to determine collective identity, which sets into motion social dynamics that lead to organized collective action. The model was tested in a series of eight studies with participants from diverse backgrounds U.S. combat veterans, college students, British football fans, Brazilian Jiiu Jitsue practitioners, twins. Overwhelming the results from these diverse samples using diverse methods showed that dysphoric experiences increased collective identity and willingness to contribute to the group through self-sacrifice.

As shown in Figure 1, groups perceiving injustice are significantly more likely to react violently and rapidly in high coordination toward groups perceived as posing external threats, especially when costs are high and regardless of group size; and groups perceiving justice do not respond strongly to external threat. These results are important because a commonly cited counterfactual is that external threats to groups that have not experienced injustice are more swiftly addressed through targeted return strikes because these groups are less chaotic, and more organized than groups experiencing injustice. In fact the embedded assumption that injustice breeds disorganization may be overly simplistic. The research by Professor Gavrilets suggests that the determining factor may be sporadic vs. chronic dysphoric experiences, with chronic dysphoria generating a common collective identity and a tendency toward self-organization in collectives, whereas sporadic dysphoria acts a shock to the system that inhibits organization and coordinated responses to threats. Additionally, Professor Gavrilets' research shows that process losses such as Ringlemann effects and groupthink are more pronounced in collectives experiencing euphoria than those experiencing dysphoria. That is, group size and underestimation of an adversarial group's capabilities are more likely in euphoric groups, even though collective identity is stronger in dysphoric groups. This explains inconsistent results across 40 years of research on in-group/out-group dynamics. It has long been theorized that collective identity is the mechanism through which group cohesiveness increases and vulnerability to groupthink

increases; yet results of experiments have been inconsistent. Professor Gavrilets' research shows that the basis for collective identity is a critical factor. The project has generated over a dozen peer-reviewed publications and Professor Gavrilets was elected as a Fellow to the American Academy of Arts and Sciences.

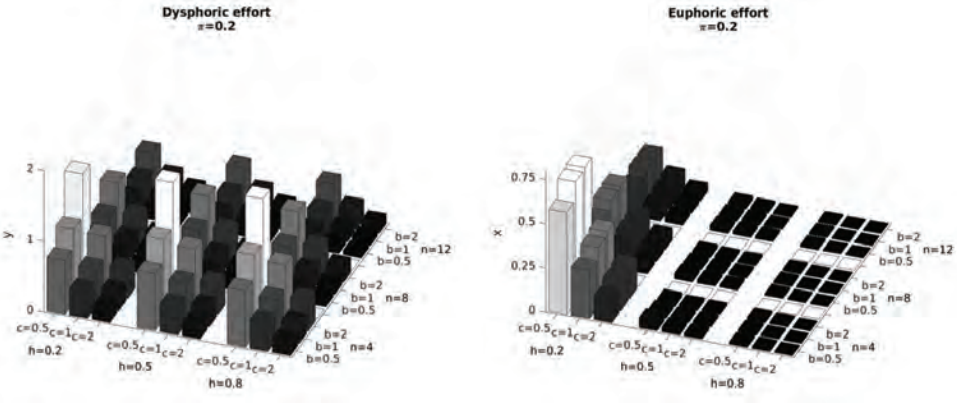


Figure 1: Effects of dysphoric and euphoric experience, group size, costs, and benefits on collective action toward external threats (Whitehouse et al., 2017; DOI: 10.1038/srep44292)

As Gavrilets' work progressed it increasingly demonstrated the importance of self-organization in coordinated collective action. His models have relied on experimental methods, enabling complete data on the membership of collectives and their attributes (including resources that they bring to the group). As noted previously, however, there is often extensive missing data in real-world groups and accurately modeling coordinated collective action in these cases has been an ongoing challenge in the social and behavioral sciences. To address this component of modeling collective action and complement the work by Gavrilets, Dr. Troyer turned to the emerging field of cliodynamics, which integrates evolutionary modeling using massive datasets that incorporate diverse data structures across multiple points in time. Cliodynamics has been developed by archaeologists and historians to leverage large databases of diverse information about cultural systems and subsystems to generate predictive macro theories of culture and social evolution, including the development of coalitions across social collectives. Prior to the rise of cliodynamics, the state-of-the-art in this domain has traditionally involved post-hoc descriptions of groups with different orientations and missions joining forces against a common external threat. While rich in detail, the historical-descriptive approach lacks the much-needed predictive capability to facilitate the prediction of how strong allied coalitions develop and mitigate the challenge of strong adversarial coalitions. A cliodynamics approach might address key to enhanced understanding of collective action, and so Dr. Troyer selected a proposal by Professor Jyette Klausen (Brandeis University) to address requirement.

Professor Klausen proposed innovative strategies based on cliodynamics to address the challenge of missing data, as in the case of dark webs – situations in which actors and groups are missing from the networks, but are often engaged in nefarious collective action. While models describing social networks of known groups are widely available, missing data characterizing influential individuals and groups has led to models that are less effective decision-making tools for analysts and leaders. Professor Klausen tackles this problem by fusing open-source media (e.g., news reports, text messages, blogs, police reports) to document violent Jihadist events in Western Europe. Using these multiple data sources, she longitudinally examined data to determine the groups and actors who left social networks, reappeared in others (often under aliases), and

moved in and out of public event reports. Decision leaders have long thought that public source data would be insufficient to track the rise and fall of coalitions among adversaries because influential collectives and actors are more opaque in social media. Using multi-urn validated algorithms with repeated bootstrap sampling across data sources to identify when actors from one collective migrated into different collectives demonstrated a pathbreaking insight: Network exits are much stronger predictors of emerging coalitions among adversarial groups than network entrances. The method also enables identification of missing links using retrospective analysis of changes in the network structure. This flies in the face of intuition, which suggested knowing who is a member of group or a coalition requires knowing when they enter the group. By treating coalition formation as dynamic processes, Professor Klausen has been able to improve on prediction and identification of key actors, including for example, the ability to distinguish lone wolf attackers from violent organizations. She also demonstrated the capability to reduce false positive identification of coalitions from 25% to 10%, providing methods to enable more rapid and accurate analyses of coalition dynamics on-the-fly.

Professor Klausen tracked 6,000 individuals involved in 797 plots with 23,000 links among persons, organizations, and events in 21 Western European nations, Canada, and United States from 1993–2016, demonstrating the formation of previously unknown coalitions, by tracking network exits, resulting in reduction in false positives from 25% to 10%. Dr. Troyer showcased Klausen's work at meetings of the National Security Administration and Department of Justice. Because of the utility of her work, the National Security Administration has extended additional funding to Dr. Klausen to increase the scope of the data collection. In addition, the Department of Justice, National Institute for Justice provided funding to extend the project to identify behavioral signs of radicalization through social media patterns of exists/entrances to coalition groups. Data from the project are publicly available through the National Archive of Criminal Justice Data, as well as the Inter-university Consortium for Political and Social Research (ICPSR). She has generated over a dozen articles in Foreign Affairs outlets, another dozen in peer-reviewed social science journals.

Result

The strategy on which Dr. Troyer has embarked to address the dynamics of collective action reflects taking on longstanding challenges for research in the social sciences by overcoming substantial deficiencies in modeling collective action. This initiative highlights the importance, dynamics, and dimensionality of collective identity as a fundamental mechanism driving collective action. Prior to this line of research, collective identity was portrayed as unidimensional and relatively stable leading to erroneous predictions about potency and persistence of action by collectives toward external threats. The research successes described here demonstrate the importance of modeling the fluidity of collective action dynamics.

The success of this research is represented in correcting longstanding model biases to generate valid depictions of collective action, as demonstrated by Professor Gavrilets' work, which incorporates realistic operationalization of collective actions as non-linear, dynamically evolving, and characterized by uncertainty within the collective regarding the resources and strategies of others. Importantly, it resolves a longstanding debate on how shared experience conditions the persistence and potency of collective action. Professor Klausen's work also incorporates a fluid view of collective identity and collective action. It refutes the persistent

Results

- Invited briefings and data/model transitions to key policymakers (Joint Staff/J9, Department of Homeland Security, Department of Justice)
- Workshop for National Security Agency with additional funding to Klausen
- Appointment of Gavrilets at American Arts and Sciences Fellow
- Over two dozen publications in diverse journals, including *Science, Royal Society, Nature Science Advances, Foreign Affairs*

inaccuracy in theory, empirical studies, and intuition that collective coalitions are stable, and in addition offers a new robust way for assessing coalition formation, with the added benefit of generating new methods to address the problem of missing data in identifying the membership and structure of violent extremist organizations. This work is already providing analysts and policy leaders with new approaches to countering violent extremism by tracking on collective experience of injustices and monitoring exits from collectives to generate predictions on the formation of adversarial coalitions.

Way Ahead

The National Security Agency and Department of Justice have received datasets and modules from the Klausen work and are working with Klausen to extend them beyond the Western Jihadist scope of the original study. The Army and broader Department of Defense community is benefiting from her work and the work of Gavrilets through briefings and workshops.

The importance of these modeling strategies for capturing the dynamic nature of collective action continues through ongoing support of the Army Research Office Behavioral Science program. The next step in this work will be to identify the drivers that distinguish between cooperation and competition among multifarious groups. If successful, this work has the potential to generate broad implications in the security, intelligence, and private sector. Understanding the factors that lead adversaries to coalesce for example, could lead to new models to detect growing threats to national security before they emerge. Also, it may provide new insights into dynamics in organizations related to mergers and acquisitions that impact trade and financial markets. As a complement to this work, Dr. Troyer is also pursuing new research on the dynamics of self-organizing systems to generate further predictive models on how groups coordinate action toward external forces to achieve disparate goals. This work may lead to new capabilities to predict the likelihood of rapid emergence of powerful threats to national security.

SUCCESS STORY

Institutional Determinants of Emergent Threats to Overmatch by Near-Peer Powers

ARO funded research resulted in **improved detection of factors** that contribute to rapid scientific development and operational transitions in near-peer powers that are challenging the U.S. overmatch in defense-related research, development, and engineering.

This success supports these ARL Core Technical Competencies:

Human Sciences

Network and Information Sciences

Challenge

Research on the tactics and strategies of near-peer powers in defense-related research, development, and engineering (R&D) is scant. Changes in the organization of science endeavors, economic incentives for science, and shifts in state politics that facilitate scientific advances in a geopolitical landscape are extremely difficult to track. Moreover, there are very different governance models, in other states such as differences in state support for the R&D enterprise, and financial and economic incentives for organizations and citizens within these states to become engaged in defense-related R&D.

This success was made possible by the following ARO S&Es or Program Specialists:

- Dr. Lisa Troyer, Life Sciences Division

Understanding how near-peer powers have advanced in defense-related R&D requires an understanding of institutional dynamics, such as how political, governance, education, and economic institutions are synchronized to advance competitive R&D. In addition, advancing this understanding requires in-depth knowledge of cultural values as they relate to both science and regime authority. Drawing on neo-institutional theory, social scientists have theorized that institutions that are structured, enacted, and described in terms of cultural values have a logic (i.e., institutional logic) that resonates with the public, giving them a taken-for-granted legitimacy. Yet, cross-cultural research examining the relationship of these factors has been sparse and examining them in the context of defense-related R&D had not been attempted until ARO embarked on this thrust. In fact, when this thrust was launched, it was possible that unifying values across institutions was a Western ideal with little utility beyond the Western world. Consequently, testing and extending the theory of institutional logics requires harnessing expertise in the local linguistic, historical, cultural knowledge of these states and integrating it with scientific and engineering advances to develop situational awareness of the advances by near-peer powers that may pose growing threats to U.S. overmatch in defense-related science, technology, and engineering.

Action

Prior to joining ARO, Dr. Troyer was engaged in studying transportation technologies that China was rapidly adopting and was also conducting research on organizational performance, legitimacy, and institutional logics. From the research on Chinese transportation technologies, Dr. Troyer observed that China was attending to the potential of transportation advances to accelerate economic growth and fuel defense-related R&D. Simultaneously, she was working with researchers who had begun to investigate Russian strategies to engage their citizens' popular support for the growth of Russia's geopolitical influence. It was also clear that the Russian strategy was tracking on the Chinese strategy: Both were aimed at enlisting citizen buy-in through an integrated strategy that appeared to fuse institutional logics and cultural values. With this in mind, upon her appointment at ARO, Dr. Troyer promptly sought scientists capable of researching the rapid social, economic, educational, and political transformations that were occurring in China and Russia, with an eye on the implications for the defense-related R&D enterprises in these states. Notably, this was a five years prior to the publication of the 2018 National Defense Strategy and The U.S. Army in Multi-Domain Operations 2028, which have since called out threats from China and Russia as they challenge U.S. overmatch in defense-related R&D. She launched the first ARO basic research initiative with emphasis on near-peer threats to U.S. supremacy in defense-related R&D by seeking projects that would provide insight on the institutional and cultural dynamics that lead to scientific advances and rapid translation of science to operations.

The key to the program on near-peer threats to U.S. defense-related overmatch was to develop scientific understanding of the institutional structure of science and how it aligns with cultural norms. Prior to beginning her appoint as program manager for the Behavioral Sciences at ARO, Dr. Troyer was an invited speaker at the annual meeting of the American Institute of Aeronautics and Astronautics session on organizational dynamics of aerospace R&D. Her talk focused on modeling sociotechnical R&D systems and led to a published paper on the complexity of sociotechnical systems and their institutional underpinnings. The research underlying the paper focused on how the unique configuration of institutions (i.e., cultural, economic, political, educational) affect national and international R&D advances. Following on her research and addressing what she perceived as rising

threats to national security in China and Russia, even before the 2018 National Defense Strategy was released citing these states as overmatch threats, she began seeking researchers who could test the advance theory-driven research on the role of institutional and cultural integration in defense-related R&D.

The first project that Dr. Troyer identified entailed work by Professor Tai Ming Cheung at the University of California – San Diego, which she recommended for support through the Army Research Office Behavioral Sciences Program. This work focused on intensive archival research in China and the U.S. using process tracing methods to track the trajectory of China's R&D developments from the 1940s the present. The project tracks development in specific domains: terrain, missile, space, aerospace, cyber, and marine.

Professor Cheung's research team demonstrated that China began embarking on a major pivot from industrial spying and reverse-engineering of Western technologies that had dominated the pre-1980s era to developing a strong institutional infrastructure that is now leading to unique Chinese-developed innovations in the defense-related R&D space that are challenging U.S. technologies. The research revealed that China is systematically and intentionally integrating education enhancements, economic incentives, political policies, and cultural marketing messaging to encourage intellectual and financial investments in defense-related R&D. For instance, the research provides the first-ever evidence that China is now incentivizing its scientists to stay in or return to China following post-graduate education to participate in state-funded R&D efforts. The incentives include state-funded laboratories, attractive salaries and benefits, and support for Chinese language scientific journals alongside incentives for publishing original research in them. In particular, the rise of Chinese-only publication outlets has hobbled the ability of non-Chinese language speakers to follow research developments coming out of research facilities in China. Also, Professor Cheung's research shows how changes in China's political regimes have fostered a capitalist pivot in the economic system that is generating economic incentives for defense-related R&D. Alongside of this, China is increasing foreign direct investment to leverage R&D by other nation states and increase access to natural resources needed to fuel its defense-related R&D. Professor Cheung's team has leveraged theories from organizational science on exploitation and exploration theories of innovation to demonstrate how China is using both strategies to absorb research by other nations, assimilate, and transform it to exploit its potential while also cultivating internal defense-related R&D to generate novel innovations and technologies. The work also highlights how Confucian values shape cultural norms that give precedence to communal efforts and motivation for perfection, which are reflected in policies of the People's Liberation Army (PLA), leading it to play a primary role in guiding control of the defense-related R&D. Prior to the 1990s, R&D in China was distributed and characterized by a "technology push" model in which PLA was a recipient of discoveries that it would then adapt for defense uses. Policies developed in the 1990s, however, transferred more control over the R&D enterprise to the PLA (facilitated by language that promoted the communal and perfection values of Confucianism), leading to a "demand pull" model. In this newer model, PLA is able to guide R&D to address state needs and fully absorb scientific advances into China's defense-related R&D.

To further scientific understanding of rapidly changing dynamics in defense-related R&D among near-peer powers, Dr. Troyer also engaged internationally recognized experts on the former Soviet Union and economies of that region. The team, led by Professor William Reisinger at the University of Iowa examined regime stability, informal economies, and economic growth. Using a transaction costs analysis framework complemented by insights

from neo-institutional theory, their research focuses on micro-scale dynamics that track how citizens are incentivized to contribute to regimes through illicit exchanges that impact regime stability and economic growth. They compared these dynamics in Russia, Ukraine, and Georgia and demonstrated that a combination of needs and opportunities affect citizens' willful engagement in illicit exchanges, such as bribery and fraud. The benefit of these exchanges, in turn, flow up regime hierarchies and are correlated with state level science and technology investments. Moreover, in stable states (characterized by infrequent regime change and lack of conflict), while illegitimate economies are less active, but not absent if individual need is high and prices in the exchange are beneficial. In unstable states, illegitimate economies are more active and viewed as normative because individual need as a justification is a culturally accepted value in each state. In both cases, individuals who engage in illicit exchanges are primarily driven by need and opportunity – lower income and opportunities to obtain goods and services lead to stronger informal economies, but the need tends to be higher in more unstable states. Professor Reisinger and his colleagues also found that in states where power is less stable and less centralized, as in the case of Ukraine vis-à-vis Russia, illicit exchanges that benefit state-led initiatives are normalized over time.

This is the first study to test the micro and macro factors that influence citizen participation in illicit economies that benefit state initiatives, including science and technology investments and the formation of economic policies. Additionally, the research represents the first test of institutional logics on informal economies and focuses on a region of profound national security interest where illicit economies pose a serious threat.

Result

The research initiative Dr. Troyer led sought to understand social dynamics and factors contributing to the growth of defense-related R&D in near-peer powers reflected her awareness of the growing challenge to U.S. overmatch in defense technologies that China and Russia were posing, well before they were called out as regions of interest in the 2018 National Defense Strategy and The U.S. Army in Multi-Domain Operations 2028. Recognizing the risks and fielding the research prior to official calls to address these rising geopolitical threats from near-peer powers demonstrates the value of basic social science research in theorizing on and identifying emerging risks at early stages and launching basic research programs to gain rapid insights.

This research initiative has resulted in confirmation of the long-held but never-tested assertion that institutional logics are a trans-cultural factor, which when consistent with cultural values, generates legitimacy that lends stability to regimes. Enterprises like R&D depend on multiple institutions: governance, educational, economic; and when these institutions are integrated (as is the case when they embody common cultural values), then the speed of discovery to operational transitions is enhanced, even if it arises through illicit exchanges. This is a substantial advance in social science theory and an enabler for additional research to examine the mechanisms that align institutional logics with cultural values. It also provides insight on potential mechanisms that may destabilize regimes, leading to conflict and disruption of global markets and alliances.

Way Ahead

Both Professors Cheung and Reisinger have briefed their project results to a number of stakeholders in the national security and national intelligence community and Professor

Results

- ARO funded research results were presented at invited briefings to Senate Foreign Affairs Committee, Department of National Intelligences, ASD(R&E), and others
- Five workshops for DoD stakeholders discussing results related to rising powers
- Briefings to United Kingdom Ministry of Defence
- Four books, six peer-reviewed journal articles

Cheung has offered multiple workshops targeted to these audiences (which are filled to capacity), demonstrating the value of the research to policy leaders and strategists.

Because of the importance of these research areas to DoD and U.S. national security, ARO is continuing to seek research that addresses factors that influence geopolitical power dynamics. The next step will entail developing a comprehensive neo-institutional theory of R&D that focuses on mechanisms through which institutions come to embody cultural values and to also investigate whether alternative factors serve the same function that cultural values provide in facilitating institutional alignment identifying. This line of research would also be advanced by investigating counter-factual cases – that is, cases where (1) institutional alignment is high, but R&D stalls; and (2) institutional alignment is low, but R&D is accelerating. This is part of a broader umbrella initiative that Dr. Troyer is developing on the social dynamics that impact scientific discovery. If successful, this would enable prediction of emerging powers long before they pose a risk or opportunity for the U.S. It will also provide insight into policies that can advance the U.S. overmatch in defense-related R&D.

Biochemistry Program

Current Scientific Objectives

01

Develop approaches to engineer and control mechanisms underlying biomolecular specificity and regulation that if successful are anticipated to lead to novel biosensing reagents and responsive materials

02

Design self-assembled biomolecular architectures to support functional organization of biological molecules that if successful are anticipated to lead to novel power and energy systems and on-site manufacturing capabilities

03

Understand sequence-structure-property relationships in biological and biohybrid materials that if successful are anticipated to lead to rationally designed materials with tailored properties ranging from therapeutics to adaptive structural materials to protect the Soldier

Program Manager

Dr. Stephanie McElhinny
Program Manager, Biochemistry
Life Sciences Division
ARO Physical Sciences Directorate

Dr. McElhinny completed her undergraduate studies at Gannon University, receiving her B.S. in Chemistry in 1999. She trained as a biochemist at the University of North Carolina - Chapel Hill, receiving her Ph.D. in Biochemistry in 2004. She came to ARO in 2009 as the Program Manager for Biochemistry.

SUCCESS STORY

Supercharging Protein Assembly for Advanced Biotemplated Materials

The ARO biochemistry portfolio enabled the **discovery of a method to drive protein self-assembly** by mixing engineered variants with opposing electrical charges, which transitioned to the ARL TRANSFORME ERP for further study into tunable materials.

This success supports these ARL Core Technical Competencies:

Protection Sciences

Materials and Manufacturing Sciences

This success was made possible by the following ARO S&Es or Program Specialists:

- Dr. Stephanie McElhinny, ARO Life Sciences Division

Challenge

Inspired by the complex structural and regulatory functions that are performed by ordered protein assemblies in nature, researchers have long sought to design synthetic structures assembled from protein building blocks that could realize new catalytic functions or serve as structural templates for advanced materials. However, the predictive design of protein assemblies presents a significant scientific challenge. Existing computational approaches are either atomistic, which consider every atom within the protein building block and are therefore limited to just a few protein building blocks, or they employ a highly simplified "patchy sphere" approach, where interactions between building blocks are encoded into a few directional, short-ranged attractive patches on the surface of a simple colloidal sphere. Limited examples of experimental success in creating synthetic protein assemblies have required painstaking and time-intensive efforts to affix molecules onto proteins to direct their assembly or to create new proteins from scratch.

Action

In 2014, Dr. McElhinny invited Professor Andy Ellington at UT – Austin and Professor Sharon Glotzer at University of Michigan to submit a white paper on a research concept that she identified as a technically bold and novel approach. In an attempt to enable protein assembly by design and surpass the limitations of both atomistic and "patchy sphere" modeling approaches, Professors Ellington and Glotzer proposed a "patchy shape" modeling approach, which would combine features of more atomistic approaches with the idea of a coarse-grained representation of protein shape with attractive "patches". Dr. McElhinny supported this research concept as a joint effort, with Professor Glotzer's group contributing the computational expertise to implement the new "patchy shape" modeling approach, and Professor Ellington's group experimentally testing the "patchy shape" model by mixing protein variants of opposing electrical charges to mimic colloidal assembly driven by shape and attractive "patches". If Professors Ellington and Glotzer were correct, and protein self-assembly could be predicted based upon the same driving forces observed for colloidal nanoparticles – particle shape and interactions between attractive/repulsive patches. Dr. McElhinny recognized the transformational impact this would have on our ability to design protein assemblies that span different length scales to realize new functions and properties not yet possible.

Result

The modeling and experimental work under this effort began in parallel. The initial results came from the experimental component, which then informed the modeling

efforts. Professor Ellington's group used a well-characterized fluorescent protein, superfolder green flourescent protein, as their model protein and generated "supercharged" variants by introducing mutations that resulted in a highly positive variant and a highly negative variant. When they mixed these oppositely charged variants, a particle formed that was distinctly larger than either of the variants alone. To explore the molecular structure of this particle, termed a "protomer" by the researchers, the team invited cryo-electron microscopy expert Professor David Taylor to join the effort. Professor Taylor successfully imaged the particles and discovered that the supercharged variants had assembled into a well-ordered, discrete ring structure, composed of two stacked octomeric rings (Figure 1). Professor Glotzer's group used this detailed structure to build an atomic model of the particle which revealed that the rings are assembled from alternating positively and negatively supercharged variants and confirmed that the interactions between the variants in the particle are mediated by the opposing charges of the variants. The high resolution structure also informed the "patchy shape" model developed by Professor Glotzer's group, enabling the model to more accurately predict the stability of the particle in the presence of salt.

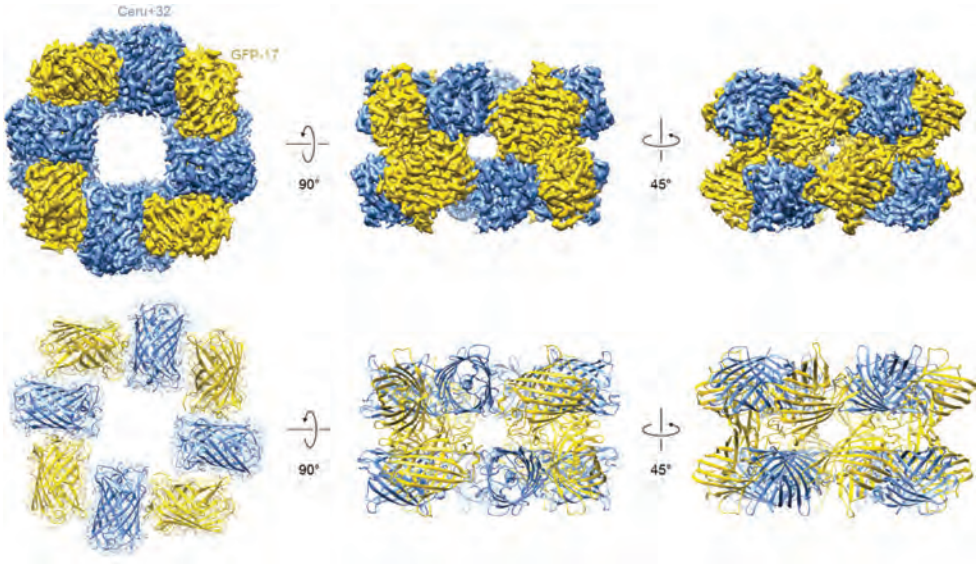


Figure 1: (Top) Cryo-electron microscopy (cryo-EM) structure of the protomer at 3.47 Angstroms resolution in three different orientations. The positively supercharged variant is shown in blue, and the negatively supercharged variant is shown in yellow. The protomer is composed of two stacked rings, each consisting of eight proteins, four positive variants alternating with four negative variants. (Bottom) Atomic model of the protomer in the three orientations corresponding to the cyro-EM structures above. Only the top ring is shown in the left panel for clarity.

During the course of the project, the new CCDC ARL site called ARL South was officially announced, and Dr. McElhinny recognized the potential of the research expertise of the Professor Ellington at UT – Austin to positively impact intramural ARL South research efforts. Dr. McElhinny proactively encouraged the Professor Ellington to explore opportunities to partner with ARL South. As a result of her initiative, a former graduate student supported by this ARO funded project was hired as an ARL South scientist.

The scientific impact of this study is a simplified approach to semi-direct protein assembly via opposing electrical charges. Moreover, the results support the team's original hypothesis that proteins can be treated as patchy nanoparticles for predictive assembly. The paper describing these results, including co-authorship by the ARL South scientist supported under this project as a graduate student, was featured on the March 2019 cover of the scientific journal *Nature Chemistry* (Figure 2).

Results

- Co-publication between Army and academic researchers in *Nature Chemistry*
- A former ARO funded academic researcher was hired by ARL to provide the Army with in-house expertise in this area
- Self-assembly approach transitioned to ARL collaborative effort with Lockheed Martin under the TRANSFORME ERP exploring programmable protein assemblies as scaffolds for materials and coatings

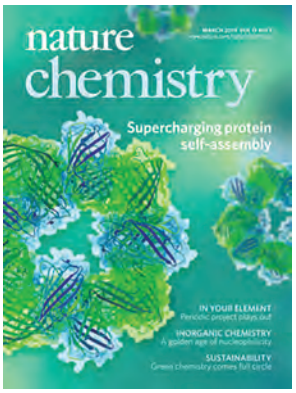


Figure 2: Supercharging Protein Self-Assembly was the cover feature of the March 2019 issue of *Nature Chemistry*.

Way Ahead

Based on the significant success of this project, Dr. McElhinny is currently supporting an extension of this effort which aims to generalize the supercharging self-assembly method to other proteins and to scale the self-assembly process from the nanometer to the micrometer size scale. If this approach can be applied to any protein of interest and scaled to sizes relevant for material systems, this could have transformational impact on our ability to design protein-based materials with new functions and properties not yet possible.

The supercharging self-assembly approach has transitioned to a new collaborative project with Lockheed Martin under the CCDC ARL to explore programmable protein assemblies as scaffolds for use in functional coatings and materials.

SUCCESS STORY

Research integrating Chemistry and Synthetic Biology led to new BioBit™ educational platform

This ARO initiative led to the **unexpected result of an educational platform** to train the next generation of scientists in synthetic biology.

This success supports these ARL Core Technical Competencies:

Materials and Manufacturing Sciences

This success was made possible by the following ARO S&Es or Program Specialists:

- Dr. Stephanie McElhinny, ARO Life Sciences Division
- Dr. Dawanne Poree, ARO Chemical Sciences Division

Challenge

The method and field of synthetic biology aims to program biological systems to carry out useful functions. This field has made meaningful progress toward the biomanufacturing of medicines, sustainable chemicals, and advanced fuels, as well as cellular diagnostics and therapies. At the core of these advances is the ability to control and tune the processes of transcription and translation, potentially offering access to non-natural materials that cannot be made by any other means. As an example, the translation apparatus is the biological cell's factory for protein synthesis. The ribosome is a molecular machine that polymerizes α-amino acids into proteins through the creation of amide bonds. It is the catalytic workhorse of the translation apparatus, with protein synthesis rates of up to 20 amino acids per second at an accuracy of 99.99%. The extraordinary catalytic capacity of the translation machinery has attracted extensive efforts to engineer it to generate other polymers beyond natural proteins.

Most research efforts in this area have focused on the site-specific incorporation of unnatural α-amino acids into proteins by the natural translation apparatus; however, the potential to engineer the ribosome to perform alternative chemistries beyond the amide bond formation remained virtually unexplored.

Action

In 2015, recognizing emerging advances in synthetic biology, and particularly the development of in vitro systems capable of modifying biological translation machinery, Drs. Poree and McElhinny conceived of a MURI topic focused on re-engineering the translation machinery to accept and polymerize non-biological monomers in a sequence-defined manner. Sequence defined polymers (SDPs) are linear macromolecules whose chemical and physical properties can be programmed with atomic-scale resolution. It has been impossible, so far, to produce finely tailored non-natural SDPs (i.e., materials of defined atomic sequence, exact monodisperse length, and programmed stereochemistry), yet the development of synthetic routes toward these molecules promises technological breakthroughs in advanced functional materials, nanotechnology, electronics, and beyond. To achieve this ambitious goal, the MURI team, led by Professor Michael Jewett of Northwestern University, proposed to develop novel cell-free biosynthetic platforms that enable the generation and evaluation of modified ribosomes and other translation factors in a non-cellular, *in vitro* setting. This dramatically expands the ribosome design space accessible to the team, as ribosomes are essential for cell viability and only limited ribosome mutations are possible in cells. While the team has made several notable advances in the development of a cell-free ribosome construction platform as well as analytical tools for single molecule characterization of SDPs, this work has made possible the serendipitous development of a modular synthetic biology educational kit that can greatly enhance the teaching of science, technology, engineering, and math (STEM) concepts while also making cutting-edge science easy to use and accessible.

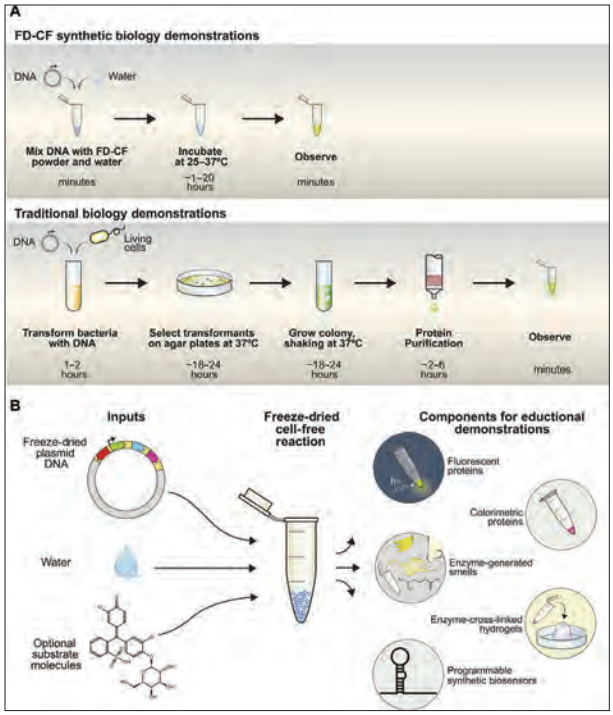
Result

The MURI team demonstrated that the cell-free systems developed as part of the MURI effort can be freeze-dried along with genetic elements to form pellets that are stable at room temperature and easily transported between team members. The shelf-stable nature of these freeze-dried, cell-free (FD-CF) pellets eliminates the need for dedicated refrigerators or freezers. In addition, FD-CF reactions do not require any specialized equipment, making them a robust technology for using synthetic biology in low-resource environments. While, from an Army perspective, this makes these systems ideal for enabling on-demand chemical production in remote environments, the unique practicality of the FD-CF technology also renders them highly suitable for applications in biology education where there is currently a glaring lack of hands-on synthetic biology experiments. To explore the FD-CF technology as an educational tool, the research team partnered with Chicago-area teachers to develop curricula for high school math and middle school science classes, to emphasize the cross-cutting nature and the value of this activity at various educational levels. The resultant BioBit™ Explorer and BioBit™ Bright kits included a set of demonstrations designed to engage three of the five senses – sight, smell, and touch – through the expression of proteins in FD-CF reactions that produce fluorescence, enzyme-generated fragrances, and large-scale hydrogels, respectively (Figure 3).

These outputs provide demonstrations that can be used to teach fundamental biology concepts and principles of tunable protein expression, enzyme catalysis, and material properties. An additional module was also created that allows students to take DNA extracted from fruit and analyze the samples using toehold switch sensors designed

Results

- Two Science Advances publications on the BioBits™ Bright and Explorer platforms
- BioBits™ Bright and Explorer kits commercialized by miniPCR bio™, now available to educators
- BioBits Bright™ has been used by ARL SEDD as part of an Army-sponsored STEM outreach program



(From left) **Figure 3:** BioBit™ educational kits based upon FD-CF technology; **Figure 4:** BioBit™ kit designed to be used by students and teachers with no biological training. Kits are also designed to be modular to allow students/teachers to design their own experiments.

to detect specific DNA sequences from the banana and kiwi genome, allowing for the first-ever student experiments that enable probing of DNA on the genetic level (Figure 4). Notably, the toolkits are designed to be modular, allowing teachers to tailor the demonstrations to their curricula. Because of the highly portable, cost-effective, and user-friendly nature of the reagents and laboratory activities, the BioBits™ Bright and Explorer kits have utility both inside and outside of a formal classroom or laboratory setting. Thus, these resources promise to increase access to cell-free technologies, enhance basic biology education, and increase participation in the field of synthetic biology which will be essential for realizing scientific discoveries in the 21st century.

Way Ahead

For the Army, research in synthetic biology will be essential for realizing scientific discoveries necessary to render next-generation advances in responsive materials, game-changing chemical, material, and drug manufacturing methods, the detection and elimination of toxic chemicals, and medical applications ranging from the detection and treatment of traumatic brain injury to the development of integrated prosthetics. If the United States is to maintain leadership in the field of synthetic biology in the coming decades, current elementary, middle school and high school students must be encouraged to pursue long term study in this field. The BioBits™ kits provide an ideal platform for teaching advanced molecular and synthetic biology concepts in a hands-on manner. The research team has already partnered with ARL SEDD to provide BioBits Bright™ as part of an Army-sponsored STEM outreach program. Beyond the educational platform, the MURI team is continuing to extend the boundaries of cell-free synthetic biology to enable re-engineering of the ribosome's active site to promote novel non-natural polymer synthesis.

Genetics Program

Current Scientific Objectives

01

Understand the molecular biology and genetics of oxidative phosphorylation and free radical leakage in order to extend the ability of Soldiers to maintain peak cognitive and physical performance

02

Understand the biology of metabolic regulation in order to reduce Soldier deaths on the battlefield

03

Create DNA based capabilities for new sources of intelligence

Program Manager

Dr. Micheline Strand
Program Manager, Genetics
Division Chief, Life Sciences Division
ARO Physical Sciences Directorate

Dr. Strand completed her undergraduate studies at Oberlin College, receiving her B.A. in Biology in 1985. She trained as a geneticist at the University of North Carolina - Chapel Hill, receiving her Ph.D. in Genetics and Molecular Biology in 1995. She conducted her postdoctoral research at the National Institute of Health. She came to ARO in 2000 as the Program Manager for Genetics.

SUCCESS STORY

Blood Chemistry and Surviving Severe Trauma

This ARO initiative resulted in the **identification of metabolic pathways that may enable future methods to reduce the risk of death after severe injury.**

This success supports these ARL Core Technical Competencies:

Protection Sciences

Challenge

How do some humans survive events that would otherwise be expected to be fatal? Humans have survived after many hours of being buried by avalanches, falling into icy water, and even traveling in unheated, unoxygenated wheel jets of trans-continental flights. These humans are often recovered being cold, apparently lifeless, and having neither a pulse nor a heartbeat. However, survival after such trauma is frequent enough that a cold pulse-less, heartbeat-less body cannot be declared dead unless it remains

This success was made possible by the following ARO S&Es or Program Specialists:

- Dr. Micheline Strand, ARO Life Sciences Division

Results

- New discoveries submitted and under review in journal *Science*
- Venture capital funding obtained for human clinical trials

lifeless after being warmed. What are the biological mechanisms allowing these phenomena, and could an understanding of this process enable its activation in a safe and controlled fashion to improve survival after severe injuries?

Action

Dr. Micheline Strand recognized the importance of high risk research ideas proposed by Dr. Mark Roth (Fred Hutchinson Cancer Research Center and the University of Washington) in studying the mechanisms of metabolic regulation and blood chemistry. Given the high Army relevance of studies in this area, Dr. Strand championed Dr. Roth's addition to the ARO portfolio. In FY19, Dr. Roth continued his investigations into the concentration of specific elemental reducing agents in the blood of rodents and humans exposed to severe trauma. The intent of this work is to identify the underlying biological mechanisms in order to develop countermeasures and therapeutics for Soldiers who receive severe blunt force trauma and other life-threatening injuries, so that fewer Soldiers die on the battlefield.

Result

Dr. Roth discovered and demonstrated that rats increase the level of a specific compound in their blood by more than twelve-fold within fifteen minutes of exposure to near lethal low concentrations (5.5%) of oxygen. He also demonstrated that this same compound increased in the blood of sepsis patients by more than thirty-fold in less than three minutes, and that humans suffering from severe blunt force trauma also increase the levels in their blood within 2.2 hours. He furthermore demonstrated that the availability of this compound within individual humans directly correlates with improved outcomes in preclinical models of ischemic injury. Preliminary data indicates that the mechanism of action is control of the trauma-triggered burst of free radicals that would otherwise permanently damage DNA, lipids and proteins.

In collaboration with Dr. Kelly Drew, Dr. Roth investigated the levels of this compound in hibernating ground squirrels and discovered that blood levels increase four-fold just prior to ending hibernation. These results are consistent with their hypothesis that this compound is a key regulator of metabolic rate.

Further work demonstrated that release of this compound in life threatening situations such as severe blunt force trauma or lethally low levels of oxygen reduces total in vivo concentrations by approximately ten percent. This compound is rare in the diets of land-based organisms such as humans and these results suggest that normal human diets may be grossly deficient in this element, and that supplementing the diets of Soldiers and civilians could profoundly improve survival after severe trauma.

Way Ahead

Dr. Strand initiated a visit by Dr. Roth to CCDC SC in January 2020 to discuss introducing this compound to Soldier rations to reduce Soldier mortality. It is anticipated that this will be a low-cost, high return on investment opportunity to significantly reduce Soldier deaths. Dr. Roth has already conducted human clinical trials which demonstrated that a 10,000 increase in blood levels is completely safe.

Dr. Roth continues to work towards commercializing this technology, with the first commercial target being protection against stroke and heart attack. Currently this work is not funded by

the Army, and has transitioned to support through other Army and government agencies with investment toward a potential protection mechanisms for hemorrhagic shock, blunt trauma, and traumatic brain injury. This path forward demonstrates how the initiative and foresight of ARO scientists continues to drive new discoveries that will impact the future Soldier.

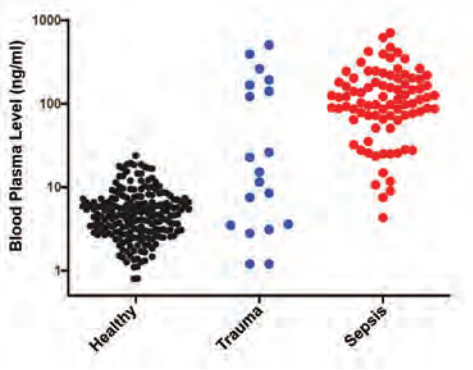


Figure 1: Plasma levels in healthy human volunteers, trauma and sepsis patients. Healthy n = 208, Mean = 5.7, SD = 4.1, SE = 0.29, Range 0.8 to 23.7; ICU/Trauma n = 45, Mean = 187, SD = 377, SE = 56, Range 1.2 to 2304; Sepsis n = 19, Mean = 196, SD = 89, SE = 20, Range = 28 to 39; T-Test comparing Healthy and ICU/Trauma using Welch's correction for unequal variance $P < 0.0024$; T-Test comparing Healthy and Sepsis using Welch's correction for unequal variance $P < 0.0001$.

SUCCESS STORY

Advancing Understanding of Neurodegeneration Using Single Cell Organisms

This ARO initiative resulted in the development of a **tractable single cell system to study the molecular dynamics of neurodegeneration**, which is linked to PTSD and a range of age-related diseases.

Challenge

Fourteen percent of U.S. veterans from recent conflicts in Iraq and Afghanistan currently have Post Traumatic Stress Disorder (PTSD). Thirty one percent of male Vietnam veterans have had PTSD and fifteen percent of Vietnam veterans currently have PTSD. Four percent of male and ten percent of female U.S. civilians will suffer PTSD in their life time. PTSD has a wide variety and range of symptoms and can mildly or completely interfere with veterans returning to normal post-duty civilian life. PTSD is linked to an elevated risk of a broad range of age-related diseases and neurodegeneration. It is believed that PSTD potentiates oxidative stress and accelerates cellular aging. The risk of developing PTSD and its impacts to the current and future Soldier are significant, yet the broad range of phenotypes and the variability in severity have been a barrier preventing scientists from elucidating the underlying molecular mechanisms of PTSD.

Action

Recognizing the incomplete understanding of intracellular control of free radicals and the underutilization of single cell eukaryotes to study complex human disorders, Dr. Strand initiated basic research to advance the Army's understanding of the intracellular molecular cascades involved in free radical mediated damage to DNA, lipids, and proteins. One component of this work resulted in the advancement of the budding yeast *Saccharomyces cerevisiae* as a tractable model system for untangling the complex pathways involved in neurodegeneration. Although *S. cerevisiae* does not have a brain, it is an excellent genetic model to explore the basic metabolic pathways involved in neurodegeneration, which are conserved between *S. cerevisiae* and *Homo sapiens.*

This success supports these ARL Core Technical Competencies:

Protection Sciences

This success was made possible by the following ARO S&Es or Program Specialists:

- Dr. Micheline Strand, ARO Life Sciences Division

Result

The ARO funded investigator Professor Antonio Barrientos (University of Miami School of Medicine) and his graduate student Andrea Ruetenik identified the critical steps for using *S. cerevisiae* in neurodegeneration basic research. First, the crucial events preceding cell death that are manifested during the course of the human disorder must be recapitulated in the *S. cerevisiae* model.

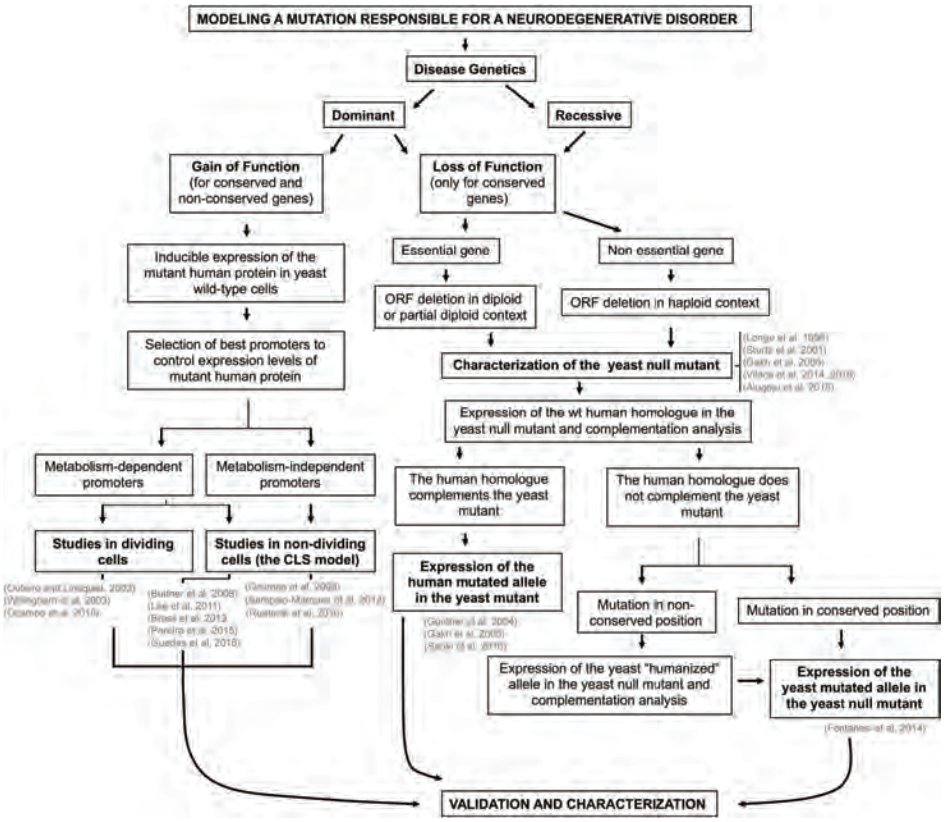


Figure 2: Modeling a mutation responsible for a neurodegenerative disorder (Ruetenik A and Barrientos A (2018) Exploiting Post-mitotic Yeast Cultures to Model Neurodegeneration. Front. Mol. Neurosci. 11:400.)

If the neurodegenerative disorder results from a loss of function of the human gene, then the *Saccharomyces cerevisiae* gene can be replaced with the human gene and functional complementation assays can be conducted to determine whether the human gene product partially or fully replaces the function of the yeast gene product. If the human gene product complements the function of the yeast gene product then specific human polymorphisms can be tested for impact. If complementation does not occur then the human polymorphism can often still be introduced into the homologous yeast gene and functional impact can be assayed. Some common human neurodegenerative disorders such as Alzheimer's disease, Parkinson's disease and Huntington's disease, involve genes that do not have homologs in *Saccharomyces cerevisiae*. Many of these causal polymorphisms involve gain of function changes in protein function and these can also be reconstituted in *Saccharomyces cerevisiae* by expressing the human disease gene in the single cell system.

Aging in the single celled *S. cerevisiae* can be measured in two ways: the replicative life span is defined as the number of daughter cells that an individual mother cell can produce, and the chronological life span is defined as the capacity to maintain viability in stationary cultures. Although *Saccharomyces cerevisiae* also does not have a gut this organism has already been used to study the mechanisms of caloric restricted lifespan

Results

- Platform technology to enable experiments to understand the molecular biology and genetic regulation of pathways involved in neurodegeneration
- This capability enables future work to develop countermeasures and therapeutics for the Soldiers and civilians with PTSD

extension, and this work has revealed that caloric restriction extends replicative life span by down regulating the signaling pathways known as Ras/cAMP/PKA, TOR and Sch9, which sense nutrients and environmental conditions, and then make executive decisions to regulate the pace of cell growth, division and life span. These same pathways regulate stress resistance and life span in larger eukaryotes such as humans.

A number of severe human neurodegenerative diseases are caused by unstable trinucleotide repeats, these diseases include Huntington's disease, Fragile X syndrome, Friedreich's Ataxia, and a number of spinocerebellar ataxias. The CAG codon expansion in Huntington's disease results in misfolded aggregating proteins and is associated with mitochondrial dysfunction, loss of mitochondrial integrity, and neuronal damage. Cloning the CAG expansion exon into Saccharomyces cerevisiae results in a faithful modeling of the protein misfolding and aggregation and Saccharomyces cerevisiae was used to identify suppressors of polQ toxicity. Saccharomyces cerevisiae was also used to investigate how the polyQ toxicity accelerates aging, and the results demonstrated that lifespan is shortened due to impairment of mitochondrial function. The Saccharomyces cerevisiae system was also used to investigate the underlying mechanisms of Freidreich's ataxia. It is known that individuals with this disease have lower levels of the mitochondrial frataxin protein but the work in Saccharomyces cerevisiae identified the impact of individual polymorphisms in the frataxin gene.

Way Ahead

Scientists funded by ARO at the University of Miami and elsewhere will use these advances to identify and characterize the basic molecular and metabolic alternations that occur during aging of post-mitotic cells such as neurons under proteotoxic stress in order to understand the etiology of neurodegenerative proteinopathies. They will determine the effect of polyQ and alpha-synuclein proteins on chronological lifespan in Saccharomyces cerevisiae and they will characterize the chronology of protein aggregation, mitochondrial function, stress resistance, intracellular reactive oxygen species levels, oxidative protein damage, and accumulation and mobilization of reserve nutrient stores. They will establish the role of mitochondrial function, reactive oxygen species signaling, and oxidative stress in polyQ and alpha-synuclein induced cytotoxicities in aged cells and determine whether manipulation of these pathways suppresses toxicity. Finally, they will explore the connections between pro-survival nutritional cues and mitochondrial functions and determine how they modulate polyQ and alpha-synuclein induced cellular proteotoxicities in chronologically aged cells.

Mitochondria are the subcellular organelles that generate energy for eukaryotes, including humans. Mitochondrial aging with a concomitant increase in the mitochondrial production of reactive oxygen species has been demonstrated to reduce life span in multiple species. Metabolic and mitochondrial abnormalities are a prominent feature of aging and neurodegeneration. Previous results indicate that mitochondrial dysfunction is an important contributor to polyQ and alpha-synuclein cytotoxicities and that these cytotoxicities can be ameliorated by the enhancement of mitochondrial biogenesis. The ability to control stress resistance mechanisms such as those against proteotoxic stress may provide molecular targets and tools to enhance warfighter performance and to prevent neurodegeneration in warfighters suffering from TBI, PTSD and other battlefield stressors.

Microbiology Program

Current Scientific Objectives

01

Discover the dynamics and communication mechanisms that drive robustness and function within bacterial communities that if successful, is expected to lead to the effective design of microbial-based platforms for on-demand fielded material synthesis

02

Develop and test experimental strategies to better understand the physiology of complex microbial communities that if successful, will provide reliable new platforms for the study of the human microbiome

03

Identify and characterize bacterial metabolic programming under harsh environmental conditions that if successful, will provide new approaches in the field of synthetic biology toward fielded living material systems that could create materials on demand for the Soldier

Program Manager

Dr. Robert Kokoska

Program Manager, Microbiology

Life Sciences Division

ARO Physical Sciences Directorate

Dr. Kokoska completed his undergraduate studies at Villanova University, receiving his B.Ch.E. in Chemical Engineering in 1978. He trained as a biochemist at Duke University receiving his Ph.D. in Biochemistry in 1995. He came to ARO in 2006 as the Program Manager for Biochemistry. He later served as the University Affiliated Research Center (UARC) Program Manager, and became the Microbiology Program Manager in 2014.

SUCCESS STORY

Bottom-up Construction of Biofilms and Microbial Community Structures

A new ARO-initiative in biofilms and microbial communities, developed in collaboration with ARO and the ARL Living Materials Essential Research Program, is driving research to explore **experimental platforms to support ARL's in house synthetic biology programs.**

This success supports these ARL Core Technical Competencies:

Materials and Manufacturing Sciences

Computational Sciences

Challenge

Living microorganisms have become an attractive platform for the reliable synthesis of a number of valuable compounds and as sentinels for the sensing of environmental contaminants. The presence of diverse microbial life in practically every environmental niche on this planet and the growing ability to engineer these microbes provides nearly limitless potential for the breadth of microbial biosynthesis and for their utilization in a number of challenging environments. Moreover, this potential can be further realized through the rational engineering of microbial communities where one can utilize more than one microbial species that work together to perform biosynthetic tasks that neither can perform alone. While metabolic modeling studies of various microbial species have provided a suitable means for identifying species that can work synergistically to perform a desired biosynthetic task, there remains a challenge to optimally control both the utilization of feedstocks and the metabolic flux of intermediates toward reliable and substantive product yield. In addition, if microbes are engineered to provide a sensing function, platform technologies are needed to impose spatial constraints to microbial deposition such that the sensing can be readily detected and amplified and where background noise is minimized.

Action

Dr. Kokoska recognized that discovering how to effectively engineer biofilms was one means of imposing spatial constraints that could overcome barriers toward the engineering of microbial communities. Traditionally, biofilms are thought to be entities that should be avoided; indeed, pathogenic microbes embedded in biofilms prevalent in hospital settings are recalcitrant to killing and dispersal thus presenting a serious health hazard. Also, biofilms present on ship hulls and fuel tanks are responsible for significant material erosion thereby limiting mission effectiveness for the DoD. In spite of these detriments, we can turn our view of biofilms on its head and recognize that microbial community engineering stands to benefit greatly by exploiting properties of biofilms. Most importantly, as opposed to microbes in a liquid culture that are well-mixed, biofilms provide spatial order to the community. Cells present in biofilms are held together by an extracellular matrix that provides non-motile deposition in the form of "molecular glue". It is also thought that the biomolecular components of this matrix impart not just a mechanical function, but also a means of efficiently channeling charge and material exchange between cells in the biofilm. Given this, it is thought that if one can effectively control deposition of one or more species into a defined spatial biofilm structure, these spatial architectures can be modeled and systematically tested for their engineered function.

Dr. Kokoska encouraged the development of white papers that would propose new thinking in the area of bottom-up biofilm design coupled with test cases that can verify the ability to control functionality. As this approach also had strong interest from the CCDC ARL Biotechnology Branch program in Living Materials, he solicited feedback from Living Materials scientists on the merits of these white papers as they pertained to the CCDC ARL program. From these partnered strategic discussions, two high quality collaborative proposals were submitted and successfully competed for FY19 Congressional funding under the Army strategic topic "Precision Controlled Synthetic Biology".

Result

Two new collaborative research efforts began in FY19 as a result of the new research initiative in biofilms and microbial communities.

This success was made possible by the following ARO S&Es or Program Specialists:

- Dr. Robert Kokoska, ARO Life Sciences Division

Results

- New program thrust that leverages new capabilities in microfluidics and 3D printing to advance discoveries in microbial community structure and function
- Ongoing collaborative research between Texas A&M University and ARL in house researchers to transition a platform to create and analyze microbial communities

1) 3D printing for directed construction of microbial biofilms.

3D printing has been recognized as a disruptive technology that can enable the creation of concise, high precision and repeatable custom-built materials. As a "layer-by-layer" deposition approach capable of assembling a broad range of materials, it has been used to produce items as broad as medical equipment, clothing, food and engine parts. As its utility is just starting to be realized for the printing of biomaterials, Professor James Wilking of Montana State University is being funded through the ARO Microbiology program to push the limits of 3D printing methodology for directed construction of microbial biofilms. Wilking's approach will be to use stereolithography (SLA)-based 3D printing where a solid object is built up layer-by-layer from a liquid resin using a focused laser spot. Polymerization of a material occurs at the laser focal point which is raster scanned within the resin bath. Here, hydrogels will be printed from a water-based resin with selective entrapment of microbes in the hydrogel in specific locations (Figure 1). The biological system under study, as designed Professor Matthew Fields of MSU, will examine how spatial deposition affects the performance of a syntrophic two-microbe bacterial-archaeal system consisting of the sulfate-reducing bacterium *Desulfovibrio vulgaris* which in the absence of sulfate as an electron acceptor, can reduce protons to hydrogen, and which can feed the methanogenic partner *Methanococcus maripaludis* to affect the reduction of CO2 to methane. Various spatial architectures will be examined including one where the alternating sections of liquid infused with one microbe are congealed, then to gel the remaining sections of the partner microbe creating a "checkboard" structure. From a series of well-controlled biofilm constructions and measurements of metabolite production, one can then assess the specific spatial features of the constructed biofilms that favor the syntrophic metabolism.

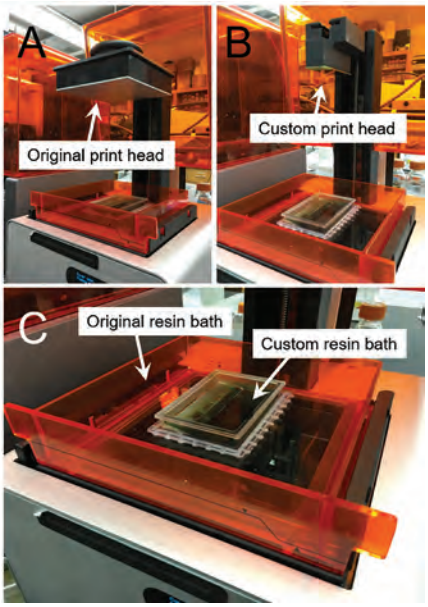


Figure 1: Modification of a commercial SLA printer for printing small hydrogels. SLA printer (Formlabs Form 1+) with the (A) original print head and with (B) a custom (3-D printed) print head with a glass slide attached. (C) A custom resin bath capable of holding resin volumes on the order of tens of milliliters is set inside the original resin bath.

2) Microfluidic-based "on-chip" platform for assembly and analysis of microbial communities.

To provide exquisite control over microbial community composition and 3D spatial organization, Professor Arum Han of Texas A&M University (TAMU) is also being funded through the ARO Microbiology program to develop a novel microfluidic-based "on-chip" platform that supports the high-throughput assembly and analysis of "designer" microbial communities in which community structure and biological function of custom-assembled microbiomes can be interrogated Here, cell-encapsulated gel micro-droplets will be the basic building block to form a complex 3D microbial community, where the biocompatible porous gel droplet allows cells to grow within the gel.

As depicted in Figure 2, using the microfluidic ARCHITECT platform, many of these gel droplets will then be assembled in a random or controlled manner to form a 2D

gel slab first and then a 3D gel block by stacking multiples of these 2D gel slabs, thus forming a spatially-defined 3D microbial community. The microbial composition and concentrations of these 2D/3D communities will be controlled microfluidically during the gel droplet assembly process. Professor Han's collaborator, Professor Paul deFigueiredo of TAMU, will develop a mathematical framework for guiding the assembly of 2D and 3D microbial communities and to use the model to generate testable hypotheses on the formation of microbial communities. The model will incorporate terms that account for cell density and describe the production, diffusion, directionality and uptake of quorum sensing signals. A subset of the data will be used to estimate model parameters and train the model, while the remaining data sets will be used for testing the model predictions. The expected model output would be testable predictions on different features of microbial community function. This modeling will guide the testing of a synthetic quorum sensing circuit built into *E. coli* cells for the assembly of microbial communities using the engineered platform. A prediction-validation approach will guide spatial formulation of communities. Similarly, model simulations will also be used to analyze and interpret data from randomly assembled communities so that underlying design principles can be elucidated.

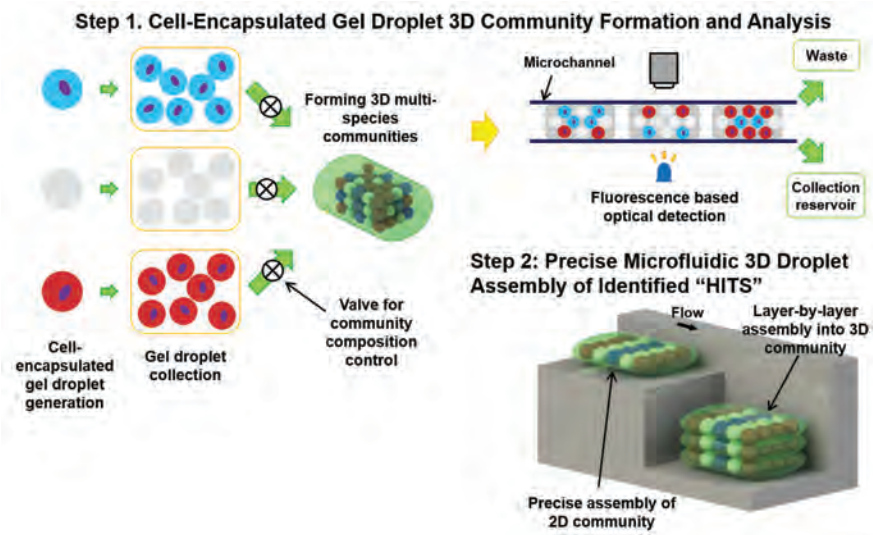


Figure 2: Illustration of the ARCHITECT platform that supports the high-throughput assembly and analysis of "designer" microbial communities.

Way Ahead

As these two collaborative research efforts are developed, findings and platform technologies will be introduced to the ARL Living Materials program and to the scientists working within the newly launched ARL TRANSFORM Essential Research Program (ERP). This ERP, with its focus on how to utilize synthetic biology to accelerate natural biological processes and to harness biology's capacity for adaptable low energy routes for material production, thus stands to benefit greatly from future collaborative work with these ARO funded investigators. The proposal led by Professor Han in particular can realize immediate value with ARL. Professor Han is also currently funded through the ERP to utilize his engineering expertise in microfluidics to perform high throughput screening of a vast array of microorganisms and sub-populations of microbial communities for their bioproduction capabilities and for identifying the characteristics that govern the interactions between various environmental microbes and inorganic surfaces. Thus, the existing relationship between Professor Han and ARL and the close link between the ARO and ARL funded projects will help facilitate a valuable transition of discoveries made through Professor Han's microbial deposition system.

SUCCESS STORY

Screening of Extremophilic Microbial Communities for New Antimicrobials

This ARO initiative resulted in the **development of a high throughput pipeline for the screening of virtually any collection of environmental microorganisms** for the discovery of antimicrobial compounds.

This success supports these ARL Core Technical Competencies:

Protection Sciences

This success was made possible by the following ARO S&Es or Program Specialists:

- Dr. Robert Kokoska, ARO Life Sciences Division

Challenge

The presence of antibiotic-resistant pathogenic microorganisms is a well-known continuing health concern and the potential for new emerging pathogens that can be packaged as biowarfare agents represents a significant threat to the Warfighter and civilian population. As antibiotic-resistant pathogens are responsible for annually killing hundreds of thousands of people worldwide, there exists a need for the development of new countermeasures with unique chemistries designed to overcome the resistance mechanisms of these "super bugs". With the increasing discovery of new drug-resistant strains of bacteria and a decline in the research and development for new antimicrobials from the pharmaceutical industry, the DoD sees a strong need to reinvigorate this field of research in order to protect the Soldier against current and emerging pathogenic threats. A significant challenge remains then for the development of novel techniques and approaches for identifying new candidate robust antimicrobials against a broad range of pathogenic threats.

Action

Many currently-used antibiotics such as penicillin and vancomycin are produced by environmental microbes. These compounds are natural metabolic by-products that are used by these other organisms as defense mechanisms against pathogenic invaders present in their environmental niche. As naturally occurring microorganisms can then be a potential source for newly discovered antimicrobials, the recent explosion of newly discovered microorganisms through the ever-expanding genomics revolution provides a virtually limitless resource for new potential antimicrobials. Indeed, most environmental samples from soils and aquatic environments house hundreds if not thousands of different microbial species. Given recent developments in the ability to genomically annotate a vast array of environmental microbes, ARO partnered with the DoD Joint Science and Technology Office for Chemical and Biological Defense in 2015 to formulate a Small Business Innovative Research (SBIR) topic entitled "Exploiting Microbiome and Synthetic Biology to Discover and Produce Naturally Occurring Antibiotics". This topic challenged the small business community to develop pipelines capable of interrogating and screening complex environmental microbiomes for new families of antibiotics derived from these complex microbial communities. Phase I of this topic set out to develop the initial screen to identify gene clusters related to the biosynthesis of antimicrobials and the development of *in vitro* assays for crude mixtures displaying an antimicrobial phenotype. During Phase II, antimicrobial components derived from against these crude mixtures will be purified and biochemically characterized and tested for efficacy against select pathogenic agents.

Results

The ARO initiative in this area led to the selection of the small business, iExpress Genes Inc., to isolate promising new antimicrobials. This research is conducted alongside investigators from the University of Oklahoma, through a current Phase II SBIR award. The environments of hot springs in El Salvador and Siberian permafrost soil were selected as the extreme environments ripe for discovering new extremophilic microbes.

The idea of working with extremophilic microbes is compelling for two reasons. First, the ability of these microbes to adapt to challenging environmental conditions suggests that their respective antimicrobial mechanisms and the chemistries that drive antimicrobial activity are likely to be unique. Second, given that the isolated antimicrobial agents will be isolated from microbes that thrive under temperature extremes, there is a high likelihood that these agents will exhibit enhanced thermal stability which can reduce the logistic burden through elimination of the need for controlled temperature storage of these reagents.

During Phases I and II of this effort, iExpress Genes developed methods for cell lysis of these environmental communities, isolated purified DNA fragments from these lysates, created a vast library of DNA clones and performed high throughput sequencing and genomic profiling of these clones to identify stretches of DNA that encode natural products. Several hundred of these candidate clones were then transformed and expressed in E. coli and subsequently screened for antimicrobial activity through plate assays. During Phase II, they successfully identified antimicrobial activity from six different natural product extracts; working with their academic partner, they have rigorously purified the activity from one select extract, performed chemical structural analysis, *in vitro* cytotoxicity tests and subsequently, partnered with at the U.S. Army Medical Research Institute for Infectious Disease (USAMRIID) to test for *in vitro* efficacy against three bacterial pathogens. The group's academic partners also synthesized a number of analogs to this isolate which are currently undergoing similar *in vitro* testing. The success of this methodology to isolate and screen candidate antimicrobials enables a continuous processing pipeline of numerous other environmental samples at iExpress Genes with the goal of expeditiously expanding the repertoire of candidate antimicrobials.

Way Ahead

Unfortunately, as USAMRIID's laboratories were recently closed, the loss of iExpress Genes' "no cost" partner, Dr. Kokoska strongly encouraged iExpress Genes to seek out new partners to perform the necessary *in vivo* efficacy and toxicity tests of their candidate compound and its analogs. iExpress Genes responded with a quality augmentation proposal to perform this facet of the research, that bring in two companies that have the necessary personnel and safety facilities as new partners. It is the goal of this collaborative group to deliver a lead antibacterial candidate with in vivo efficacy toward further advancement for the submission of an Investigational New Drug application with the U.S. Food and Drug Administration.

Results

- Collaborative small business effort resulted in the isolation of several promising environmental microbial extracts that demonstrate antimicrobial activity.
- Subsequent purification of one promising antimicrobial candidate led to the design and synthesis of a battery of analogs that can be readily screened for enhanced antimicrobial activity.
- The DoD Joint Science & Technology Office (JSTO) for Chem Bio Defense provided supplemental funding to support the necessary *in vivo* tests of these analog compounds.
- Army support of this effort has provided a ready-made platform for the continuous screening of a virtually unlimited suite of environmental microbe collections to further identify and purify new antimicrobials.

Neurophysiology of Cognition Program

Current Scientific Objectives

01

Map, measure and model structural and functional neural components of multisensory synthesis and modulate human multisensory information processing bandwidths that if successful, is expected to lead to new methods to optimize learning, cognitive resilience, and peak performance in complex multi-domain operations

02

Determine how brains structure, process and refine biological neural networks to generate efficient decisions and behaviors that if successful, is expected to lead to new training methods, equipment design, and paradigms for human-machine teaming

03

Determine underlying neurobiological mechanisms mediating the vulnerability of the brain to mild injury under high-rate loading conditions that if successful, is expected to lead to new methods to prevent and treat traumatic brain injury

Program Manager

Dr. Frederick Gregory

Program Manager, Neurophysiology of Cognition

Life Sciences Division

ARO Physical Sciences Directorate

Dr. Gregory completed his undergraduate studies at Morehouse College, receiving his B.S. in Biology in 1999. He trained as a Neurobiologist at the University of California - Los Angeles receiving his Ph.D. in Neurobiology in 2006. He came to ARO in 2013 as Program Manager for Neurophysiology and then took on the additional role of International Program Manager for Human Dimension in 2016.

SUCCESS STORY

New Tool for Seeing the Inner Workings of the Brain

ARO-supported research has contributed to the goals of the White House BRAIN Initiative; **new tools for bio-imaging enable super-multiplexed images of brain cells**.

This success supports these ARL Core Technical Competencies:

Human Sciences

Challenge

In 2013 President Barack Obama announced the launch of the White House Brain Research through Advancing Innovative Neurotechnologies (BRAIN) Initiative, which has since led to an ambitious private-public partnership aimed at revolutionizing our understanding of the human brain. The initiative was motivated by several years of research and reports from scientists and professional societies that indicated a clear need for innovative experimental tools to help neuroscientists tackle many of the basic mysteries of the brain. As a result, many federal agencies, private research institutes and academic institutions have partnered to realize the dream of the White House's initiative and is anticipated to do for neuroscience what the Human Genome Project did for genomics.

DARPA has been the primary Department of Defense organization that has made coordinated investments contributing to the mission of the BRAIN Initiative. After five years of investments, DARPA has fostered revolutionary scientific opportunities through development of new neurotechnologies that might enable novel deep brain stimulation-based treatment of neurological disorders, a brain prosthetic for memory and transcranial stimulation to improve consolidation of learned information while we sleep. CCDC ARL ARO Neurophysiology of Cognition program manager, Dr. Frederick Gregory, co-managed several research projects supported through the DARPA BRAIN effort and has also made strategic investments to enable new neurotechnologies to address scientific barriers facing the Army of 2050.

Action

The ARO's BRAIN-related investments are multidisciplinary efforts varied across experimental platforms that range from imaging and recording the electrical activity of neurons in-vivo to transcranial stimulation. One scientific barrier addressed by these investments is an essential need for the ability to directly visualize a large number of distinct molecules inside living neurons to understand complex processes related to behavior and performance. Professor Wei Min from Columbia University approached ARO with a team of leading researchers, led by Professor Rafael Yuste from Columbia, to address the need for new tools to image structure-function relationships in the living brain. Professor Min brought years of experience working with Raman Spectroscopy to the task of making the technique compatible to biological systems. This tactic was one of several different approaches chosen by the research team to address the objectives of the ARO Simultaneous Multi-Synaptic Imaging of the Interneuron MURI; just prior to President Obama's BRAIN Initiative announcement in 2012. The goal of this MURI is to understand how individual neurons act as computational elements by developing the capability to visualize structure-function across the hundreds to thousands of a living neuron's synapses. Traditionally, fluorescence microscopy is one method of choice for live-cell imaging, but limitations (mainly spectral spread) prevent imaging more than 2-5 different molecules with high selectivity and sensitivity under biological conditions. Professor Min's objective was to advance the Raman scattering technique to overcome these limitations and enable the capability to simultaneously image over 25 different colors simultaneously in a biological preparation.

Raman scattering spectroscopy (SRS) is a technique used for imaging the vibrations of individual chemical bonds (Figure 1). Since the invention of SRS microscopy, imaging molecules without specific labels or tags (label-free imaging) has been a

This success was made possible by the following ARO S&Es or Program Specialists:

- Dr. Frederick Gregory, ARO Life Sciences Division

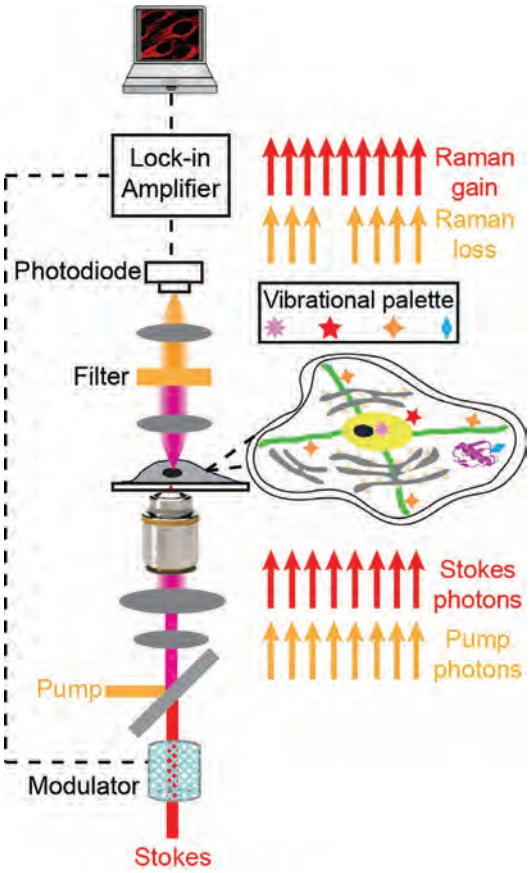


Figure 1: SRS microscopy. A narrow-band pump laser (6-ps pulse width) and an intensity modulated Stokes laser (fixed at 1064 nm, 6-ps pulse width) are both temporally and spatially synchronized before focusing onto cell samples. When the energy difference between the pump photons and the Stokes photons matches with the vibrational frequency (ωvib) of the targeted chemical bonds, the chemical bonds are efficiently excited to the vibrational excited state. For each transition, a photon in the pump beam is annihilated (stimulated Raman loss) and a photon in the Stokes beam is created (stimulated Raman gain). A lock-in detection scheme is used to sensitively measure the intensity loss. doi: 10.1038/nature22051

central theme of its application. Despite the popularity of this idea in biomedicine, the strategy has limitations preventing application to understanding the living brain. The main challenge is the difficulty to distinguish one target biomolecule of interest from the many other related species inside cells since many biomolecular species share similar chemical bonds. Professor Min's solution was to combine contributions from advances in spectroscopy and chemistry to create orders-of-magnitude more sensitive and mutually resolvable vibrational 'tags' for simultaneous specific labeling of biomolecules. Professor Min's research effort sought to test basic hypotheses about the chemistry underlying these vibrational tags and generate a large library of novel vibrational tags. Proof-of-principle observations were going to be made utilizing these new probes for understanding the intricate biological environment and activities of living tissues. Coupling SRS with strong vibrational tags such as alkynes (C≡C) allows effective imaging of diverse biomolecules, but detection sensitivity is limited to about 15 mM for typical chemical bonds such as C–H and 200 μM for the stronger C≡C bond, leaving many targets (such as metabolites, proteins, RNA and organelles) out of reach. This new work extends Raman scattering from a pure spectroscopic to microscopic technique, in which the sensitivity could reach down to 250 nM with maintained fine selectivity.

Results

This research effort sought to couple advances in stimulated Raman scattering microscopy with newly designed and synthesized vibrational probes to achieve much enhanced detection sensitivity. By installing triple bonds (e.g. C≡C and C≡N) and other chemical modifications onto the light-absorbing chromophores of the tags (Figure 2), a wide spectrum of well-resolved chemical colors was obtained for "super-multiplex vibrational imaging". In tandem with fluorescence imaging, 30 colors could be obtained for imaging multiple biological targets in complex biological samples at one time. It was estimated that the newly developed tools offer about 1,000 times more sensitivity than the previous record for stimulated Raman scattering imaging and is demonstrated to show sensitivity comparable to that of confocal fluorescence microscopy. A major outcome of this new development was the exquisite vibrational selectivity of the probes, thus allowing previously unachievable high number of colors that could be simultaneously imaged.

Results

- Discovery of super-multiplex vibrational imaging method that offers sensitivity, high resolution and biocompatibility; enabling a new era in bioimaging to probe and identify previously hard to study phenomena
- Generated a research tool that paves the way for deeper insights into the molecular bases of human performance, synthetic biology applications and in material sciences

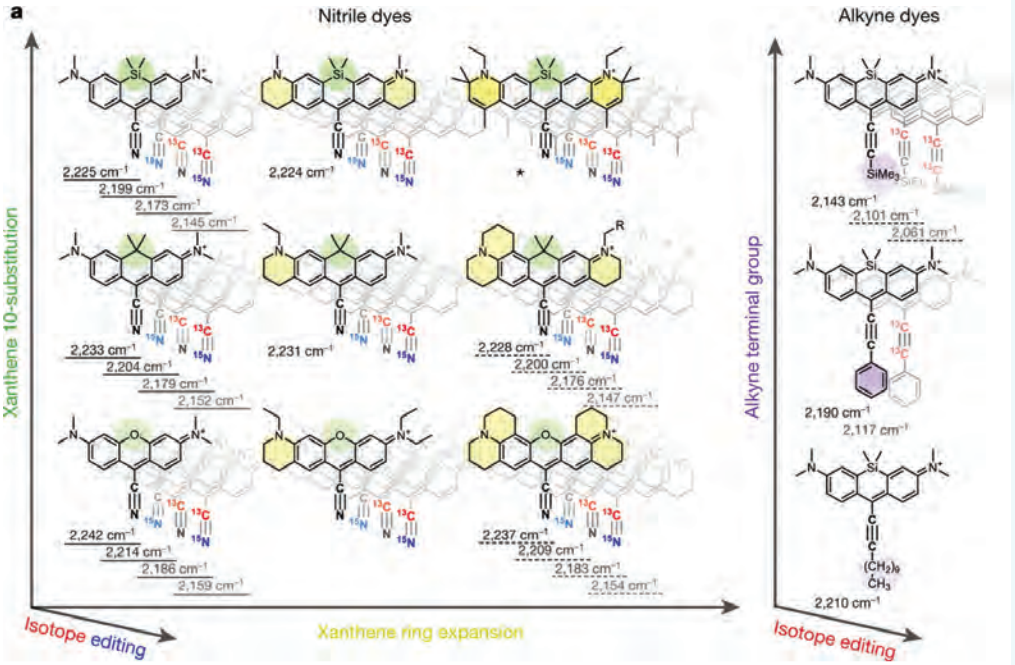


Figure 2: Design principles and structures for a library of epr-SRS nitrile and alkyne dyes. doi: 10.1038/nature22051

Way Ahead

Super-multiplex vibrational imaging offers sensitivity, high resolution and biocompatibility. The major breakthrough offered by this study is that the multiplex labeling versatility of this approach exceeds the existing multiplexing optical ceiling. When combined with available fluorescent probes, the array of currently available vibrational probes developed provides 30 resolvable colors, with the potential for further expansion. Super-multiplex vibrational imaging may be applied to interrogate and potentially offer new biological insights into complex biological processes such as long-term memory formation or blast-induced traumatic neurotrauma in which molecular metabolism and interaction is critically involved, yet hard to study. Transitions to industry could also leverage the high biocompatibility of these vibrational probes for therapeutic imaging or clinical diagnostics in humans, in the near future.

SUCCESS STORY

Emerging View of Vascular Control in the Brain

ARO research led to **development of an optical imaging system** to peer at the interactions between blood vessels and neurons in the living brain at the University of Wisconsin-Milwaukee

This success supports these ARL Core Technical Competencies:

Human Sciences

Challenge

The ARL ARO Neurophysiology of Cognition program supports broad approaches to decipher the neural codes underlying human perception, sensorimotor integration and behavior. One specific scientific barrier being addressed is understanding the intricate

Results

- Developed multi-modal optical technique based on optical coherence tomography that allows simultaneous imaging of blood vessels and nearby neural network activity in the living brain
- Created new paradigm for studying coupling between vascular activity and neural networks paves the way for broader understanding of brain function and potential neurovascular-based metric of cognitive performance

interaction of neurons with glia and blood vessels. Lack of basic knowledge on how neurons, glia and blood vessels integrate into functional brain circuits is a fundamental barrier to understanding cognitive performance and, ultimately, limits solutions that effectively enable heightened Soldier rapid decision-making, cognitive control and mental agility. Understanding the mechanisms that mediate this coupling will provide greater insights into the brain's information processing pathways and the role of brain states in mediating cognitive performance. The program is addressing this barrier by advancing neurotechnology development to generate new capabilities to map, measure and model neurophysiological-hemodynamic interactions at near-cellular levels.

Action

The Neurophysiology of Cognition program manager, Dr. Gregory, presented a new scientific opportunity during the 2015 Life Sciences Board of Visitor division review to focus on an emerging area of coupling between blood vessel dynamics (hemodynamics) and neuronal dynamics. However, the experimental tools to obtain simultaneous imaging of both features was limited. Dr. Gregory, strategically invested in DURIP instrumentation in 2016 to permit Professor Ramin Pashaie at University of Wisconsin to assemble a spectral-domain optical coherence tomography (SD-OCT) imaging system to potentially overcome the technical hurdle (Figure 3).

SD-OCT is a versatile imaging technique with the ability to acquire 3D images at a resolution as low as 2 μm up to several hundred micrometers deep in a scattering tissue, like the brain. Despite commercial OCT scanner development and the wide range of applications, modifications of this technology can require complex optical designs or custom-machined parts that increase the ultimate cost of the SD-OCT setup; precluding its use by many researchers. In order to overcome this barrier, the DURIP investment allowed the University of Wisconsin team to build a versatile system that could be integrated with other optical technologies. The cost-effective design was then made available to the academic community. Researchers leveraged this new capability and combined OCT imaging with simultaneous optogenetic neurostimulation to activate specific neuronal activity, and test interactions between neural activity and local blood flow. Recent research demonstrated deep brain imaging of vasculature morphology in the rat brain, corresponding to the entire depth of the cerebral cortex. Patterns of optical neurostimulation were then applied to the cortex of transgenic optogenetic mice blood flow-rate, velocity, and diameter changes of selected middle cerebral artery branches were measured.

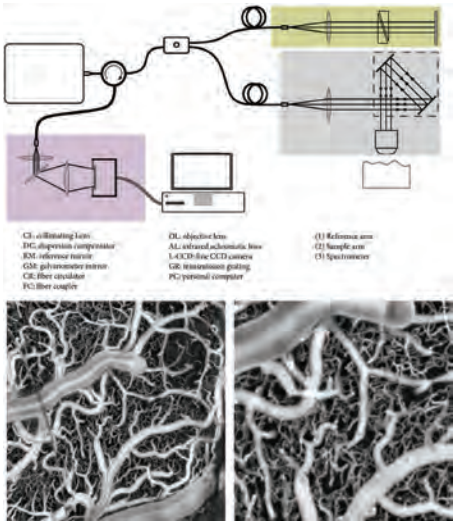


Figure 3: Top, Design of the new optical fiber-based SD-OCT system. The system uses a low coherence light source to launch light into sample (path 2) and reference (path 1). Light that is collected back from the reference and sample paths recombines to form interference patterns detected by spectrometer (path 3). Bottom, Preliminary DURIP-funding results of SD-OCT imaging of capillaries in rat brain. doi: 10.1155/2018/3726207

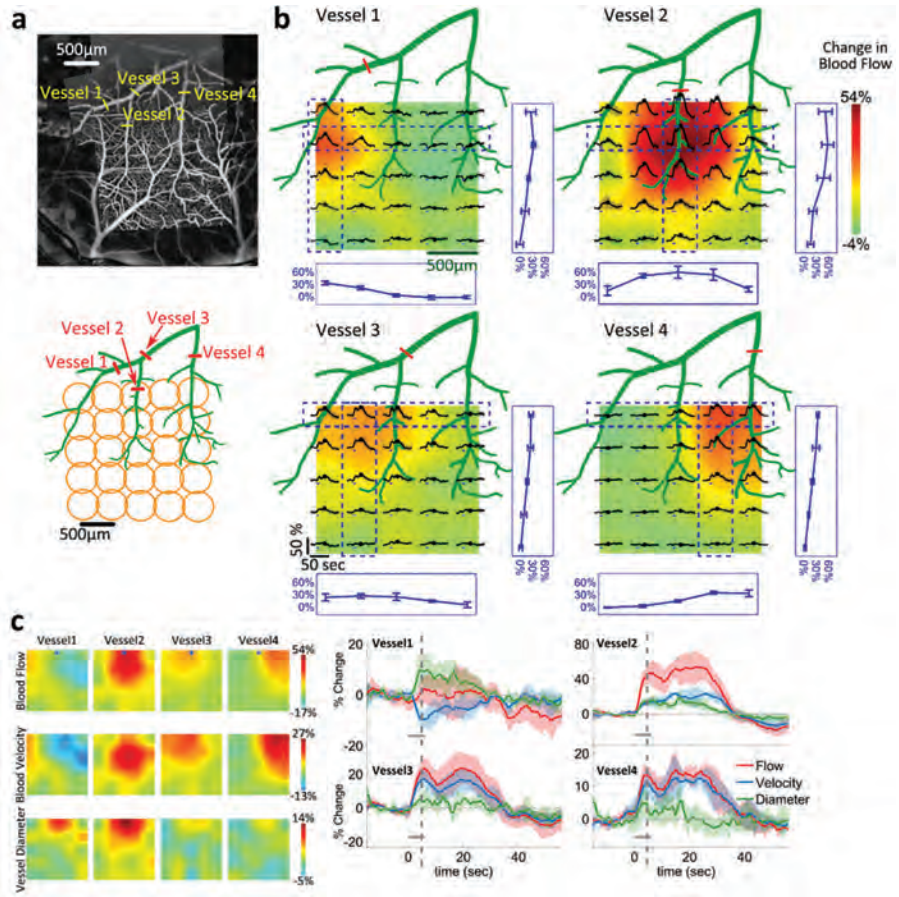


Figure 4: Result of simultaneous OCT and optogenetic stimulation demonstrated the existence of vascular 'receptive fields'. Left. The vascular network in the animal under test (top) and the 25 stimulation locations (bottom) in a form of a 5 by 5 matrix. Diameters of the circles are 461 µm to represent the actual beam diameter on the tissue surface. The red lines mark the vessel cross-sections that are imaged as monitoring sites. Right. The color-coded receptive field (RF) of the arterial blood flow for the four selected vessel cross-sections. The dark red color shows strong increase, green color represents zero response, and blue color represents decrease in the blood flow-rate in each vessel. The recorded blood flow-rate response in each stimulation location is displayed in the color-coded image. The side panels for each receptive field represent the measured increase in blood flow-rate at the marked rows and columns. doi: 10.1088/1741-2552/aad840

Interestingly, neuronal stimulation relative to the surrounding vasculature had notable effects on vasodynamic response patterns (Figure 4). Generally, neural stimulation in the vicinity of downstream capillaries of an artery evoked a fast increase in the blood flow-rate, velocity, and vessel diameter. When neural stimulation was delivered in the vicinity of one daughter branch of an artery, they observed a drop in blood velocity and/or flow rate along with increase of the vessel diameter.

Way Ahead

This technical achievement paved the way for studying correlations and causal relationships between blood vessel dynamics and nearby neural activity. This pioneering outcome opens new lines of research with potential applications in understanding fundamental cerebrovascular regulatory principles linking neuro-glio-vascular coupling to information processing and brain states, which will be important to consider within the context of future brain-based training and performance enhancement strategies as well as for potential to inform a new class of more robust bio-inspired artificial neural network architectures.

Atomic and Molecular Physics Program

Current Scientific Objectives

01

Investigate many-body quantum systems to discover new phenomena that can be exploited for novel capabilities in metrology, computation, material design, and communication

02

Drive scientific inquiry into new regimes of physics to enable discoveries in entanglement that can expand knowledge of physical constraints of computation and sensing, with anticipated future applications ranging from covet sensing to resilient communication systems

03

Achieve control for state-to-state chemical reactions, quantum state preparation, and intermolecular interactions that if successful, will enable future technologies to protect the Soldier and Army network, such as the selective detection of chemical threats at range, synthetic routes to new energetic materials, and to support applications in quantum computing

Program Manager

Dr. Paul M. Baker
Program Manager, Atomic and Molecular Physics
Physics Division
ARO Physical Sciences Directorate

Dr. Baker completed his undergraduate studies at Wright State University, graduating with Honors with a B.S. in Physics in 2002. He trained in atomic physics at the Tufts University, receiving his Ph.D. in Physics in 2009. He came to ARO in 2010 as the Program Manager for the atomic and molecular physics (AMP) program.

This success supports these ARL Core Technical Competencies:

Network and Information Sciences

Materials and Manufacturing Sciences

Computational Sciences

SUCCESS STORY

Demonstration of Non-Trivial Topological Properties in Graphene

ARO funded studies demonstrated **exotic insulating phases in twisted bi-layer graphene**, providing potential new paradigm toward new physical platforms for topological quantum computing and sensing.

Challenge

Taking advantage of quantum processes requires balancing the need for control and complexity with the deleterious effects of noise which grows with system size. Current platforms go to tremendous lengths to isolate and protect qubits, which are atoms or artificial atom-like structures that can hold quantum information, from the environment. Theoretical studies have suggested that some systems that can support quasiparticles called non-abelian anyons, which have fundamentally different interactions with their environment and with each other. These quasiparticles are immune to errors caused by local noise sources and are ideal candidates for quantum sensing and computation tasks. A few experimental systems have emerged such as ultracold atoms in optical lattices and layered 2D materials that may serve as platforms for non-abelian anyons. These are nascent concepts and illumination at this point requires experimental exploration on multiple systems as well as an extensive theoretical effort.

Action

Dr. Paul Baker, ARO atomic and molecular physics (AMP) program manager (PM) held a Workshop in Dallas Texas in 2013 to explore potential research paths for topological matter. After some initial theoretical funding, Drs. Baker and Ulrich recognized that the studies could answer complementary questions of interest to the objectives of the ARO AMP and Condensed Matter Physics programs. Drs. Ulrich and Baker then held a second workshop specifically on anyons in 2015 to determine the current challenges in the field with potential impact to both ARO programs. The two ARO PMs then conceived of a joint Multidisciplinary, University Research Initiative (MURI) topic on anyonic matter in cold atomic and condensed matter systems that was ultimately selected by OSD, and later awarded to the UCSB team led by Professor Andrea Young.

The MURI team was comprised of several theorists, three ultracold atom experimental groups and two experimental groups that would investigate the properties of graphene. Graphene is a two dimensional semimetal that had shown hallmarks of the fractional quantum hall effect which is an indication of non-abelian anyons. Collaboration between cold atomic and solid state experiments focuses on common quantum simulations and models as well as a number of cross-fertilizing ideas, including new ways to engineer optical lattices and entropy measurements in solid state systems.

Within a short period of time members of the MURI team have made significant progress. Cold atom groups are investigating different ways to realize nontrivial topological phases by creating novel optical traps. At Rice University, Professor Randy Hulet studies topological excitations in a 1D quantum gas, while at Berkley, Professor Dan Stamper-Kurn is producing topological insulators in 2D kagome optical lattices. In condensed matter systems, Professor Young and researchers at UCSB and team member Professor Cory Dean at Columbia University have been exploring Hall effects in graphene. While there are many successes to report, the results reported in journal articles *Tuning superconductivity in twisted bilayer graphene* [*Science* 363, 1059 (2019)] and *Large linear-in-temperature resistivity in twisted bilayer graphene*, [*Nature Physics* 15, 1011 (2019)] have been the most exciting results thus far and demonstrate the potential of this material to engineer phenomena of interest such as anyons.

This success was made possible by the following ARO S&Es or Program Specialists:

- Dr. Paul M. Baker, ARO Physics Division
- Dr. Marc Ulrich, ARO Physics Division

Result

Twisted bilayer graphene (TBG), as its name suggests consists of two layers of graphene stacked on top of each other at a relative angle (twist) between their lattice structures. Twisting any two lattices relative to one another will create interference patterns, with periodicity larger than the original lattice structure. These moiré patterns depend upon the twist angle and create additional symmetries that lead to interesting new physics in graphene. For example, TBGs exhibit non-trivial topologies resulting in strongly correlated electron systems. Recent results show that at a so called "magic angle" of ~1.1° the energy of electrons is virtually independent of momentum, or to say it another way, the electrons have an effectively infinite mass. Researchers outside the MURI found by merely engineering the atomic structure a nominally resistive material, carbon, is made to superconduct. This seminal result has spurred a firestorm of studies into this TBGs, whose remarkable versatility includes not just several superconducting phases but various topological insulating phases as well.

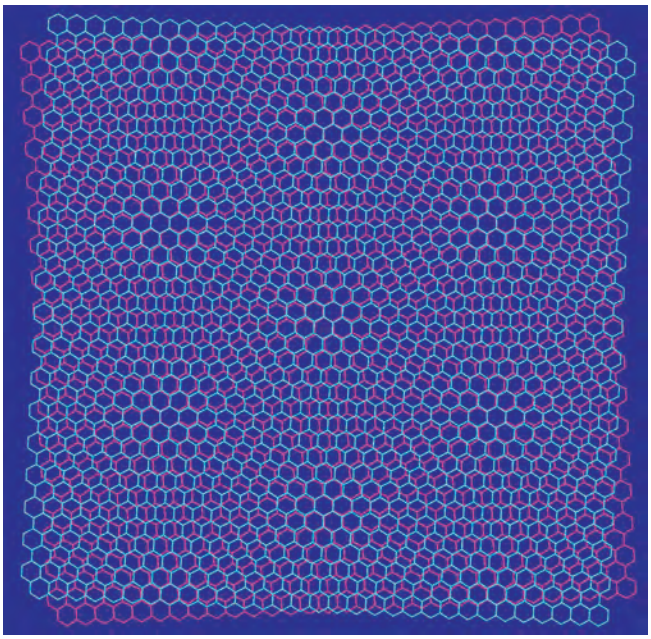


Figure 1: Overlaying the two honeycomb lattices of graphene (or any two dimensional hexagonal material) and creating a relative twist between them results in a new pattern with a longer-wavelength periodicity. This simple twist transforms carbon into a material that exhibits physics only previously observed in complex compounds with much heavier and more expensive elements and reveals new phenomena never before seen in any material.

The MURI team took this initial discovery and began mapping a more complete phase diagram in a bid to determine the origin of the effects. Most importantly, the team revealed that by adding external pressure the superconductivity in TBG could be made more stable. The range of twist angles where the superconductivity was observable was increased and insight into effects of disorder were obtained. This has given valuable information about the origin of the superconductivity in this system which remains a mystery. This advance is a particularly valuable contribution to the MURI because it represents a solid state system which can be widely tuned, similar to cold atom systems. The importance of being able to explore such a rich parameter space – twist angle, carrier density, magnetic field, pressure, interlayer distance, temperature and gate electric field to name a few – cannot be overstated. Much like ultracold atom experiments which are prized for their ability to model diverse physical system, the many parameter knobs in TBGs allow for fine control and comparisons to theory otherwise unavailable and will be important for engineering non-abelian anyons for quantum systems protected against environmental noise. Further, this allows a richer cross-fertilization between the experimental cold atom and condensed matter initiatives within the MURI.

Results

- Discovery that twisted bilayer graphene is a versatile material system for engineering new quantum materials that are otherwise unavailable
- Demonstration of direct electrical control of a new form of magnetism
- Results published in *Science and Nature* and heavily promoted in popular science publications
- ARO is supporting purchase of additional scientific equipment and expanded theoretical effort

By experimentally walking TBGs through parameter space and developing a corresponding theoretical understanding, the MURI team has uncovered other aspects of superconductivity and strongly correlated electron systems. This understanding may help guide the search for new superconductors at high temperatures which would alleviate the need for cryogenics. Further, it may lead to the development of new quantum materials with protected topological phases that could be used for quantum computation or sensing. In this very early stage the exciting possibilities are only increasing.

Way Ahead

Studies of twisted bi-layer graphene are still in their infancy. Experimental and theoretical efforts are proceeding apace. Improvements in fabrication with a focus on improving the spatial homogeneity of the TBG moiré pattern would greatly improve signal to noise in experiments. The same experimental techniques that enable twisted bilayers provide a way to construct more complex multilayer systems. One interesting possibility is the twisted double-bilayer. This four-layer system has a relative twist between two untwisted bilayers, and it is expected to have flat bands whose properties depend on an even wider range of tunable variables compared with simple TBGs. With each new advance in our understanding, and every new experimental observation comes with a host of new questions. The only certainty is that new and exciting physics will be discovered the research presses forward.

SUCCESS STORY

Demonstration of Non-Trivial Quantum Speed-up

This ARO investment resulted in the **development of a quantum system with sufficient depth to run Army relevant scheduling algorithm** that is not possible on a classical computer.

Challenge

There are a variety of important computational problems that scale exponentially with problem size. These intractable problems limit both solutions of practical problems, such as scheduling, logistics, cryptography, and scientific discovery. With the development of Shor's algorithm for reducing the computational requirements of determining prime factors of large numbers, quantum computing provides hope that additional algorithms can be found for other computationally hard problems. Some problems, however, are best managed by quantum emulation. That is, a real physical system may map precisely onto a classically computationally intractable problem of importance. Cold atomic systems are natural platforms for quantum emulations. Each atom is exactly the same – a perfect qubit – and the systems are extremely flexible. Interactions among the atoms can be mediated through lasers and entanglement can be distributed throughout arrays of atoms leading to practical realizations of quantum models. Significant technical challenges remain in implementation however, and significant research is required to realize these atom-based simulators.

This success supports these ARL Core Technical Competencies:

Materials and Manufacturing Sciences

Computational Sciences

This success was made possible by the following ARO S&Es or Program Specialists:

- Dr. Paul M. Baker, ARO Physics Division
- Dr. Sara Gamble, ARO Physics Division

Action

In the year 2015, Dr. Baker met with Professors Vladan Vuletic (MIT) and Misha Lukin (Harvard) to discuss a new method of computing with cold neutral atoms. Dr. Baker invited a Single Investigator proposal to demonstrate a proof of principle experiment titled "Novel states of light and matter mediated by collective Rydberg excitation." This investment by the ARO Atomic and Molecular Physics (AMP) Program focused on developing the tools to trap cold atoms in optical tweezers and exciting the atoms into Rydberg states. It was believed at the time that Rydberg atoms if sufficiently coherent, could be used as a new type of quantum simulator. After some initial trial and error, significant progress was made and in 2018 a new single investigator project was solicited and awarded in 2019 titled "Efficient light-matter interfaces for Rydberg arrays and entanglement in topological quantum networks." It was during these two projects that significant technical challenges were overcome and significant demonstrations made. These demonstrations resulted in DARPA's Defense Sciences Office establishing a new program titled Optimization with Noisy Intermediate-Scale Quantum devices (ONISQ). DARPA selected the team led by Professors Vuletic and Lukin as a center piece for this new program and sought out ARO's Dr. Baker and Dr. Gamble to participate in its execution. The goals of this new DARPA project will be to demonstrate computational gains beyond what is possible in a classical system, and with a focus on DoD relevant problems.

Result

The research efforts had the challenging goal of creating a physical platform that would use the quantum properties of neutral atoms for useful quantum simulation such as the maximum Independent set (MIS) algorithm. The MIS algorithm is based in graph theory and can be used to optimize scheduling tasks of importance to the DoD mission. As quantum systems grow in size (i.e. the number of qubits) decohering effects such as environmental noise can mitigate any potential advantage in growing system complexity. To address this difficulty, Professors Vuletic and Lukin chose to use 87RB atoms excited to a Rydberg state, but needed to demonstrate a precise experimental control, sufficient isolation for long lifetime coherent states, and the basic building blocks of quantum optimization such as the ability to generate entangled states.

In their experiments, individual 87Rb atoms are trapped using optical tweezer micro-traps and arranged into defect-free arrays. Deterministic loading of arrays of up to 50 micro-traps has been demonstrated in comparable systems. Coherent interactions between the atoms are enabled by exciting them to a Rydberg state. The experimental protocol consists of loading the atoms into a tweezer array and then rearranging them into a preprogrammed configuration. The final state is then detected using fluorescence imaging. The flexibility of the system is such that atoms can be trapped in arbitrary configurations. The lack of control of such traps prevented quantum emulation for many years. The recent development of optical tweezer-based micro-traps is a key technological enabler for quantum emulation.

Generation of quantum entanglement amongst many qubits is challenging because such states are extremely fragile. Despite these challenges, Professors Vuletic and Lukin demonstrated "Schrödinger cat" states with up to 20 qubits in and published the results in a co-authored journal article *Generation and manipulation of Schrödinger cat states in Rydberg atom arrays*, [*Science* 365, 570 (2019)]. In practice, the time necessary

Results

- DARPA has provided major investments in this research areas that can impact the ARL SEDD Rydberg atom group
- Academic researcher created new tools for the ARL SEDD Rydberg atom group
- Developed low power optical arrays for cold atom sensors and computers

Figure 2: (A) Single-atom-resolved images before (top) and after (bottom) rearrangement. Defects are identified, and the loaded traps are rearranged. (B) Two instances of successfully rearranged arrays (first two pictures), and one instance where a defect is visible after rearrangement (last picture). (C) The arrangement is flexible – non-periodic arrangements and adjustable lattice spacings are also possible. (D) High-resolution CCD image of trap array. [Science 354, 1024 (2016)]

to prepare such a state grows with system size and becomes prohibitively long for large N. Therefore, optimal control methods were developed to prepare precisely defined arrays as quickly as possible. By using these states to distribute entanglement to distant sites the researchers have establish important ingredients for quantum emulation and quantum metrology. This method can be extended so that the entangled atoms can remain trapped and maintain their quantum coherence over very long times. This could enable the sophisticated manipulation of entanglement for applications such as quantum optimization.

Way Ahead

Future conflicts against technological peer nations will require new capabilities to provide opportunistic overmatch. The successful demonstration of quantum systems that can efficiently perform intractable problems would provide new capabilities. Specifically, systems that can process large data sets at the point of collection can provide distributed networks with the ability to react within the decision loop of the enemy, in contested areas. The demonstration and manipulation of Schrödinger cat states in Rydberg atom arrays continues the experimental progress in a potentially useful near-term quantum system designed to tackle scheduling problems and resource allocation. In addition to providing a demonstration of useful problem, the ability for quantum systems to definitively provide solutions to problems unavailable to classical computers represents a new era of information processing. A fielded distributed networks of high-fidelity quantum sensors and quantum data processing will provide important capabilities on the U.S. Army's ability to conduct multi-domain operations.

Condensed Matter Physics Program

Current Scientific Objectives

01

Understand the physics governing the interaction between topological and magnetic states that if successful, is anticipated to lead to electronics with ultra-low power requirements to provide increased mission duration, reduced battery carry weight, and improved signature management for the Soldier

02

Unambiguously realize anyons and control them that if successful, is anticipated to lead to novel electronic functions and a new highly scalable quantum information system for new computational capabilities to protect the Army network

03

Observe new non-equilibrium states of solid state matter induced by coherent light that if successful is anticipated to open the door to new types of materials with a range of previously inaccessible structural and electronic properties that will enable the next generation of electronics for the future Soldier

Program Manager

Dr. Marc Ulrich

Division Chief, Physics Division

Program Manager, Condensed Matter Physics

Program Manager (Acting), Optical Physics and Fields

ARO Physical Sciences Directorate

Dr. Ulrich completed his undergraduate studies at Houghton College, receiving his B.S. in Physics in 1994. He trained as a physicist at Auburn University, receiving his Ph.D. in Condensed Matter Physics in 2001. He came to ARO in 2003 as the Program Manager for Condensed Matter Physics and was promoted to the additional role of Division Chief, Physics Division, in 2008.

This success supports these ARL Core Technical Competencies:

Materials and Manufacturing Sciences

Computational Sciences

SUCCESS STORY

New Instrumentation to Reveal Obscured Electrical Hall Currents

ARO funded research enabled the **development of a new electrical measurement method** that provides previously inaccessible knowledge to unique functionality in advanced electronic materials.

Challenge

A host of discoveries in electronic materials are emerging through studies of the interaction of electrical currents with magnetic fields. The most renowned of these interactions is the Hall effect in which a magnetic field causes a current through a material to be deflected perpendicular to the bias and many discoveries over the decades have been made possible with this technique – most notably the quantum and fractional quantum Hall effects. More recently, the quantum anomalous Hall effects in which currents flow without resistance around the edge of a sample – with no magnetic field. But this technique is not without difficulties and to date, for insulating samples, measurements must rely on a mathematical transformation which involves dividing by nearly zero. This means very noisy data and exciting phenomena can easily be obscured by it.

Action

While at a scientific meeting regarding private sector funding of basic research, Dr. Ulrich held a sidebar with two renowned researchers, Drs. Kapitulnik and Yacoby of Stanford and Harvard Universities respectively, to discuss an opportunity for new instrumentation for studies of advanced electronic materials. For decades, the Hall effect which was discovered in 1879 has been used to discover new phenomena involving the behavior of electrons in semiconductors and other electronic materials (Figure 1). The Hall effect is a measurement of a voltage between two sides of a sample perpendicular to the direction of current being driven through it. Naturally, this voltage would be zero but a perpendicular magnetic field will push electrons perpendicular to the driving current and cause a measurable voltage in the transverse direction. Two Nobel prizes have been awarded based on physics discovered using measurements of the Hall effect.

Two common problems arise in highly resistive samples, though. First, a slight mis-alignment of contacts on opposite sides of the sample allow a longitudinal voltage to be picked up as an artifact in the transverse measurement. Simple methods involving symmetry (flip the magnetic field) allow this artifact to be cancelled out – except when the sample is not particularly conductive. Second, if the transverse conductivity is the quantity of interest for discovering new phenomena, the mathematical procedure for extracting it involves division by nearly zero such that the measurement error diverges.

During Dr. Ulrich's meeting, the two researchers proposed a new measurement technique that would overcome these challenges and enable new discoveries. While other funding agencies had declined to support the proposition, Dr. Ulrich recognized the value of the technique should it be successful and its relevance for advancing the physics that was currently being pursued within the ARO Condensed Matter Physics program.

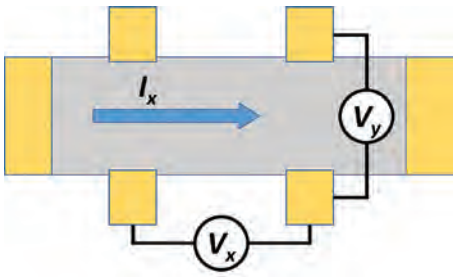


Figure 1: Traditional measurement of the Hall effect. A current, I_x, is driven longitudinally across a bar-shaped sample (grey) and both longitudinal, V_x, and transverse, V_y, voltages are measured. In a magnetic field penetrating the sample (in or out of the page), the Lorentz force will divert electrons into the transverse direction resulting in a measurable transverse voltage.

This success was made possible by the following ARO S&Es or Program Specialists:

- Dr. Marc Ulrich, ARO Physics Division

Result

The investigators proposed a technique that relies on a circular "Corbino" geometry (Figure 2).

Figure 2: The Corbino style measurement of the Hall effect. The longitudinal current is driven between the inner and outer rings in the presence of a penetrating magnetic field. The Hall effect causes a circular current around the sample and between the contact rings. (Left) This creates a magnetic moment, b, which can interact with an externally applied field, B. The interaction can be readily measured using a cantilever and techniques commonly employed in atomic force microscopy. (Right)

In the Corbino geometry, there are no contacts for the transverse voltage but the corresponding transverse (Hall) current will circulate around the sample creating a magnetic field. The researchers calculated that a cantilever and standard techniques for measuring deflection of cantilevers used in atomic force microscopy provide a sufficiently accurate measurement of the Hall effect.

After two years of effort, Drs. Kapitulnik and Yacoby succeeded in being able to use the technique to measure the Hall conductivity of a highly resistive sample directly - without resorting to troublesome mathematical transformations.

Way Ahead

Though many standard enhancements to improve the sensitivity by orders of magnitude are yet to be employed, the team has already demonstrated the ability to detect the Hall effect in samples in which traditional Hall measurement techniques struggle. Drs. Kapitulnik and Yacoby will continue their efforts to maximize the sensitivity of the technique. Once achieved, they will employ it to measure the Hall effect in several systems where it has not been possible to date.

It is expected that the technique will be adopted by many groups worldwide and advance the community's understanding of various kinds of Hall effects in advanced electronic materials. The technique may also be employed by the Service Labs as they have begun a collaborative effort on topological device concepts. The physics that can be revealed by the new technique may apply directly for these concepts.

Results

- The development of a new scientific technique which provides access to previously inaccessible physical phenomena.

SUCCESS STORY

Demonstration of Non-Trivial Topological Properties in Graphene

ARO funded studies **demonstrated exotic insulating phases in twisted bi-layer graphene**, providing potential new paradigm toward new physical platforms for topological quantum computing and sensing.

Challenge

There are a variety of important computational problems that scale exponentially with problem size. These intractable problems limit both solutions of practical problems, such as scheduling, logistics, cryptography, and scientific discovery. With the development of Shor's algorithm for reducing the computational requirements of determining prime factors of large numbers, quantum computing provides hope that additional algorithms can be found for other computationally hard problems. Some problems, however, are best managed by quantum emulation. That is, a real physical system may map precisely onto a classically computationally intractable problem of importance. Cold atomic systems are natural platforms for quantum emulations. Each atom is exactly the same – a perfect qubit – and the systems are extremely flexible. Interactions among the atoms can be mediated through lasers and entanglement can be distributed throughout arrays of atoms leading to practical realizations of quantum models. Significant technical challenges remain in implementation however, and significant research is required to realize these atom-based simulators.

Action

Dr. Paul Baker, ARO atomic and molecular physics (AMP) program manager (PM) held a Workshop in Dallas Texas in 2013 to explore potential research paths for topological matter. After some initial theoretical funding, Drs. Baker and Ulrich recognized that the studies could answer complementary questions of interest to the objectives of the ARO AMP and Condensed Matter Physics programs. Drs. Ulrich and Baker then held a second workshop specifically on anyons in 2015 to determine the current challenges in the field with potential impact to both ARO programs. The two ARO PMs then conceived of a joint Multidisciplinary, University Research Initiative (MURI) topic on anyonic matter in cold atomic and condensed matter systems that was ultimately selected by OSD, and later awarded to the UCSB team led by Professor Andrea Young.

The MURI team was comprised of several theorists, three ultracold atom experimental groups and two experimental groups that would investigate the properties of graphene. Graphene is a two dimensional semimetal that had shown hallmarks of the fractional quantum hall effect which is an indication of non-abelian anyons. Collaboration between cold atomic and solid state experiments focuses on common quantum simulations and models as well as a number of cross-fertilizing ideas, including new ways to engineer optical lattices and entropy measurements in solid state systems.

Within a short period of time members of the MURI team have made significant progress. Cold atom groups are investigating different ways to realize nontrivial topological phases by creating novel optical traps. At Rice University, Professor Randy Hulet studies topological excitations in a 1D quantum gas, while at Berkley, Professor Dan Stamper-Kurn is producing topological insulators in 2D kagome optical lattices. In condensed matter systems, Professor Young and researchers at UCSB and team member Professor Cory Dean at Columbia University have been exploring Hall effects in graphene. While there are many successes to report, the results reported in journal articles Tuning superconductivity in twisted bilayer graphene [*Science* 363, 1059 (2019)] and Large linear-in-temperature resistivity in twisted bilayer graphene, [*Nature Physics* 15, 1011 (2019)] have been the most exciting results thus far and demonstrate the potential of this material to engineer phenomena of interest such as anyons.

This success supports these ARL Core Technical Competencies:

Network and Information Sciences

Materials and Manufacturing Sciences

Computational Sciences

This success was made possible by the following ARO S&Es or Program Specialists:

- Dr. Paul M. Baker, ARO Physics Division
- Dr. Marc Ulrich, ARO Physics Division

Result

Twisted bilayer graphene (TBG), as its name suggests consists of two layers of graphene stacked on top of each other at a relative angle (twist) between their lattice structures. Twisting any two lattices relative to one another will create interference patterns, with periodicity larger than the original lattice structure. These moiré patterns depend upon the twist angle and create additional symmetries that lead to interesting new physics in graphene. For example, TBGs exhibit non-trivial topologies resulting in strongly correlated electron systems. Recent results show that at a so called "magic angle" of ~1.1° the energy of electrons is virtually independent of momentum, or to say it another way, the electrons have an effectively infinite mass. Researchers outside the MURI found by merely engineering the atomic structure a nominally resistive material, carbon, is made to superconduct. This seminal result has spurred a firestorm of studies into this TBGs, whose remarkable versatility includes not just several superconducting phases but various topological insulating phases as well.

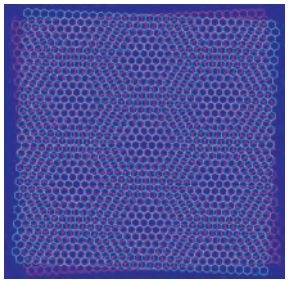


Figure 3: Overlaying the two honeycomb lattices of graphene (or any two dimensional hexagonal material) and creating a relative twist between them results in a new pattern with a longer-wavelength periodicity. This simple twist transforms carbon into a material that exhibits physics only previously observed in complex compounds with much heavier and more expensive elements and reveals new phenomena never before seen in any material.

Shortly thereafter, another group of researchers found that when this TBG was aligned with hexagonal boron nitride (hBN) in a particular way hysteretic effects emerged in the electrical transport demonstrating the presence of a new form of magnetism. This magnetism results from the orbital motion of the electrons – no magnetic moments exist in the material! High quality graphene, including TBG, is known to host topologically non-trivial phases suitable for non-abelian anyons in the presence of a magnetic field. This naturally posed the question: can this new form of magnetism play the role of an external magnetic field? The effect has been seen with other naturally magnetic materials and is known as the quantum anomalous Hall effect (QAHE). The MURI team took this initial discovery and began pursuing an answer to this question. The heroic experiments provided in two exciting results. First, the proposed QAHE was observed and second it was shown that this state can be controlled with an electric field. The impact of this result is twofold. First, much like ultracold atom experiments which are prized for their ability to model diverse physical system, the many parameter knobs in TBGs allow for fine control and comparisons to theory otherwise unavailable and will be important for engineering non-abelian anyons for quantum systems protected against environmental noise. Second, this electrical control of magnetism may provide a new route to efficient classical electronic computational schemes.

Results

- Discovery that twisted bilayer graphene is a versatile material system for engineering new quantum materials that are otherwise unavailable
- Demonstration of direct electrical control of a new form of magnetism
- Results published in *Science and Nature* and heavily promoted in popular science publications

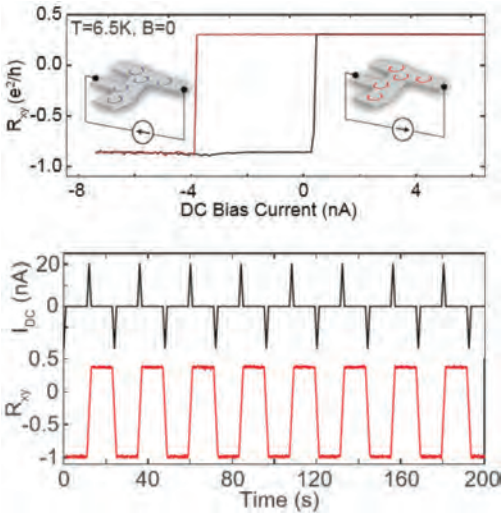


Figure 4: Electrical control of orbital magnetism. Top panel: hysteresis of electrical resistance as a function of the bias. The otherwise independent-of-current resistance is due the quantum anomalous Hall effect which is induced by the orbital magnetism of the TBG/hBN heterostructure. The magnetism is represented by the circular orbits. Note that the direction of this magnetization is readily switched by the direction of the current. Bottom panel: Once the magnetism is induced, it is stable. The current is not necessary to maintain it. (arXiv:1907.00261)

Way Ahead

Studies of twisted bi-layer graphene are still in their infancy. Experimental and theoretical efforts are proceeding apace. Improvements in fabrication with a focus on improving the spatial homogeneity of the TBG moiré pattern would greatly improve signal to noise in experiments. The same experimental techniques that enable twisted bilayers provide a way to construct more complex multilayer systems. One interesting possibility is the twisted double-bilayer. This four-layer system has a relative twist between two untwisted bilayers, and it is expected to have flat bands whose properties depend on an even wider range of tunable variables compared with simple TBGs. With each new advance in our understanding, and every new experimental observation comes with a host of new questions. The only certainty is that new and exciting physics will be discovered the research presses forward.

Optical Physics Program

Current Scientific Objectives

01

Develop non-Hermitian optics to create more sensitive optical detectors that if successful, will enable the next generation of sensors, communication, and computing devices for the future Soldier

02

Apply supersymmetric optics to develop new capabilities ranging from eliminating optical loss in sensing and communication devices to developing more powerful laser systems

03

Design, create, and understand the optics of epsilon near zero (ENZ) materials, which have very large nonlinear properties and may enable enhanced communication applications for the Army network that are more resilient to interference and require less power

Program Manager

Dr. Marc Ulrich

Division Chief, Physics Division
Program Manager, Condensed Matter Physics
Program Manager (Acting), Optical Physics and Fields
ARO Physical Sciences Directorate

Dr. Ulrich completed his undergraduate studies at Houghton College, receiving his B.S. in Physics in 1994. He trained as a physicist at Auburn University, receiving his Ph.D. in Condensed Matter Physics in 2001. He came to ARO in 2003 as the Program Manager for Condensed Matter Physics and was promoted to the additional role of Division Chief, Physics Division, in 2008.

SUCCESS STORY

Photonic Routing

ARO funded researchers developed a **photonic router that provides exquisite control of the movement of photons (light)**. This achievement will be essential for the development of future photonic computers that could replace the current paradigm of electronic computers.

This success supports these ARL Core Technical Competencies:

Network and Information Sciences

Materials and Manufacturing Sciences

Computational Sciences

This success was made possible by the following ARO S&Es or Program Specialists:

- Dr. Marc Ulrich, ARO Physics Division
- Dr. Richard Hammond (Retired), ARO Physics Division

Challenge

Integrated photonic devices have long promised significant technological advantages. Utilizing photons in replace of electrons in devices has the potential to improve sensor performance, provide near instantaneous computation upon detection for improved response times, reduce the power cost of computation, information transfer and information storage, and enable super-dense information coding. However major roadblocks to these capabilities exist in terms of the size of current platforms as well as our ability to minimize crosstalk and photonic scattering losses arising from disorder. The result reported here marks a major milestone addressing these issues.

Action

The former ARO Optical Physics and Fields program manager, Dr. Richard Hammond (now retired) had a long standing interest in the fundamentals behind integrated photonic devices. Development had stalled and a major breakthrough was needed to advance the technology. By attending and funding conferences and workshops Dr. Hammond became aware of the emerging and yet underfunded theoretical ideas regarding how equations that have solutions involving imaginary numbers can enable the control of light in fundamentally new ways. For decades, these equations were not thought to be meaningfully applicable to optical phenomena.

More specifically, Dr. Hammond considered how non-Hermitian Hamiltonians (controlling equations without real solutions) could be utilized to control light and optical fields in fundamentally new ways. In 2016, Dr. Hammond championed Dr. Liang Feng for a Young Investigator Program (YIP) grant to study these ideas. His thoughts on the matter were that the optical physics and fields program was entering a new exploratory line of research based on these equations and the corresponding physics. He envisioned optical systems that explored the interplay between loss and gain in photonic materials. By exploring these fundamental questions he felt that research breakthroughs had the potential to lead to new photonic materials and devices that would in turn lead to new ultrasensitive and/or ultra-light sensors and detectors that could help the warfighter detect threats from greater distances and lighten the pack.

Result

A primary aspect of Dr. Feng's work was to connect these equations with imaginary solutions to "topological" photonics. A topological photonic system is a periodic array of photonic elements in which the relationship between the elements is designed in such a way that that photons within cannot communicate with those without. By positioning

Results

- High profile publication in journal *Science* reporting the reconfigurable routing of optical pathways through a compact, energy efficient periodic photonic structure.

regions with different topological properties (topology) next to each other, photons can only travel along the edges of the regions and the bulk of the material and they do so with remarkable efficiency.

Under the right conditions, the topology of a system opposes the effects of disorder, hence topological protection. Additionally, changing the local nature of the topological structure can provide added functionality not seen in homogeneous bulk material. When the topology changes and is subdivided into regions, edge states can exist at the interface between the two regions. This allows for channels of electromagnetic transport within the bulk material. A breakthrough made by Professor Feng was that the topology of various regions in a large photonic system can be modified by an external laser. This provides a way to externally shuttle photons through the photonic lattice in arbitrary ways.

While edge states due topology are a phenomena that has been previously investigated – even with regards to inhomogeneous regions of topology, Professor Feng's breakthrough research provides flexible, on-the-fly re-configurability. The photonic array's topology is locally controlled by optically pumping distinct regions. By altering the pattern of light projected on the device, the edges channels are altered in turn. The pattern can be made arbitrarily complex and include multiple turnings. The result promises advances in integrated photonic device components. Complex photonic circuits would be able to process and transmit light in a manner similar to how electronic integrated circuits process and transmit electronic signals. This will lead to information moving faster and more efficiently, while using less power.

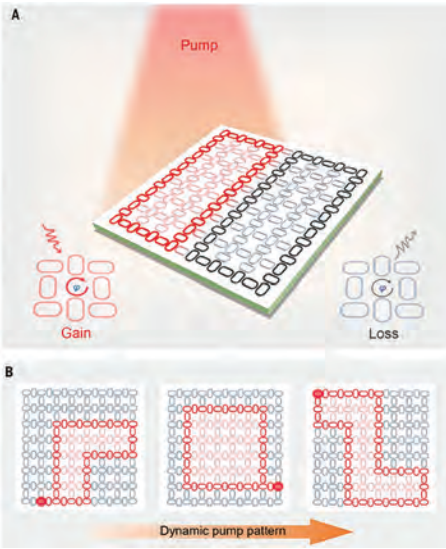


Figure 1: A) Scheme of laser-induced topological change, which creates new edge channels along the interface in the bulk of the photonic lattice with illuminated (red) and dark (black) plaquettes. (B) Topological edge states can be dynamically reconfigured to steer light along any boundaries defined by the arbitrarily patterned pump beam. [*Science* Vol. 365, Issue 6458, pp. 1163-1166].

Way Ahead

Photons move at light speed and can carry and transmit great amounts of information while releasing only a fraction of the energy they carry. In comparison, electrons are slow and far less efficient. If successful, integrating more photonic devices in micron-scale proximity on a computer chip will enable more of its components – transistors, memory, modulators, and detectors – to work seamlessly together.

Professor Feng has been awarded a 3 year single investigator grant that began in May 2019. His efforts will continue to explore new ways to control light in integrated photonic devices. Other investigations are under way into fabrication methods to incorporate photonic components into chips using the same tools used in existing fabrication facilities for electronic circuit. This will reduce cost and increase device development cycles. Another path forward is to further miniaturize these devices. Theoretically these structures can be on the scale of the wavelength of the photon utilized. Such miniaturization would further decrease the footprint and energy cost of these devices by an order of magnitude.

SUCCESS STORY

Supersymmetric Laser Arrays

ARO funding leads to **discovery that laser arrays engineered to contain specific defects harness the principles of supersymmetry** to produce efficient, high energy, and spectrally pure laser beams.

This success supports these ARL Core Technical Competencies:

Materials and Manufacturing Sciences

This success was made possible by the following ARO S&Es or Program Specialists:

- Dr. Marc Ulrich, ARO Physics Division
- Dr. Richard Hammond (Retired), ARO Physics Division

Challenge

Achieving a more intense laser beam with finer spectral quality has been an ongoing challenge in laser physics. This is because with increased power comes increased application space and spectral purity is essential for sensing and communication applications. Efficiency is also important and it will reduce the size of devices making them easier to deploy. However, there are fundamental limiting factors such as material damage thresholds that will deteriorate laser stability and the spectral quality. For solid state lasers it was assumed that stacks or arrays of lasers coupled together would result in increased beam power. While this works to a point, instabilities owing to cross-talk and interference eventually places limits on the benefit one gets from this method. Notions of "supersymmetry", a powerful mathematical procedure first developed in the context of theoretical high energy physics, has supplied optics researches with a blueprint to avoid these deleterious effects. This article focuses on the successful application of supersymmetry based laser arrays that utilize lossy array elements to generate efficient, high-power and diffraction-limited laser beams.

Action

Supersymmetric Optics is a very new field, pioneered by Professor Demetrios Christodoulides, and his team at the University of Central Florida. In 2016, Dr. Hammond held a two-day workshop at ARO where new fundamental ideas in supersymmetric optics with potential Army applications were discussed. Professor Christodoulides' research effort flows from the topics discussed at this workshop and relies on theoretical work funded elsewhere by the ARO Optics program. Dr. Hammond was very excited by this work, and has stated that this research has the potential to initiate a new subfield within Optical physics and engineering.

At the time ARO began supporting Professor Christodoulides' research, the ideas were very new and considered high risk. Therefore, Dr. Hammond send this particular research proposal for evaluation by six experts, and each gave a perfect score. One evaluator summarized the experts' perspectives: "The degree of novel ideas, good science, and talented researchers is just exceptional." The three year single investigator proposal was enthusiastically funded in 2017 and has rapidly been producing significant scientific advancements.

Result

Professor Christodoulides' ARO funded research provided a completely novel way to design optoelectronic elements. The principles of the mathematical powerhouse, supersymmetry (SUSY), opens a new design space for important functionality in counterintuitive ways. The physical world is comprised of two types of fundamental particles – those that do not interact at all and those that interact strongly. The SUSY theory demonstrates that each particle in each category has a partner (called a superpartner) in

the other. This symmetry was found to map mathematically onto gain and loss in optical systems. Thus intentionally including loss in an optical system could be beneficial to gain in other parts of the system. Employing this notion, Professor Christodoulides designed and created an array of lasers – a SUSY laser array. The main array intended for gain and lasing was created with a nearby lossy superpartner designed in such a way that undesirable laser modes would be suppressed. This allows more energy input into the system be captured by the desired laser mode.

Professor Christodoulides prepared two arrays: the SUSY laser array and one without the lossy superpartners. When illuminated at the same pump intensity level, the peak intensity produced by the SUSY array is 4.2 as high as that from the standard laser array. In the SUSY arrangement, all higher order transverse laser modes – which are undesirable and the bane of laser design – are suppressed in favor of the fundamental mode. In the far-field, the diffraction profiles reveal a pronounced difference in the SUSY laser. The far-field of the SUSY laser displays a single bright spot and has a much smaller divergence angle. This low divergence behavior is characteristic attribute of a laser array operating only in its lowest order mode. In February 2019, Professor Christodoulides' team published these results in a paper entitled "Supersymmetric laser arrays" in the journal *Science*.

Optical components in both electronic and photonic systems are vital to the warfighter. Devices utilizing high power lasers will be made more deployable. The basic principles of SUSY may also be applied to passive component, technology appearing in sensors and communications, for example. This research will develop fundamentally new ways to control light, enabling lighter more efficient devices which can lighten the warfighter's load, as well the possibility of developing totally new functionalities, such as capabilities at new wavelengths.

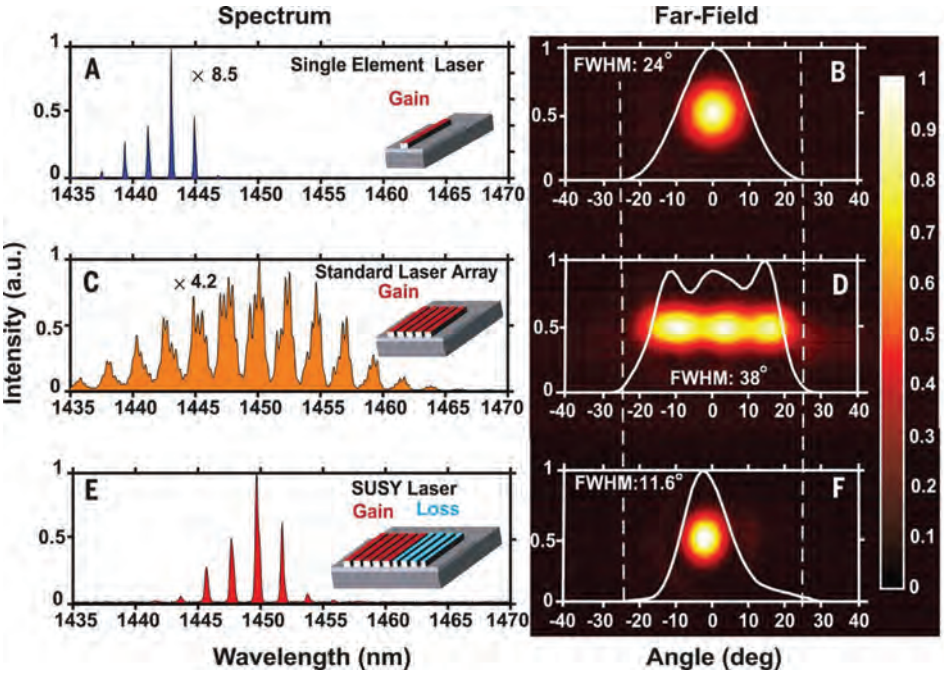


Figure 2: Spectral and far-field characteristics of the SUSY laser array. (A, C, and E) Emission spectrum of (A) a single laser cavity, (C) a standard five element laser array, and (E) a corresponding SUSY laser arrangement. The spectrum of the SUSY array is free from undesired resonances, indicating that all higher order modes are suppressed. (B, D, and F) far-field diffraction patterns from the corresponding lasers. The measured direction angle associated with the SUSY laser (~5.8°) is smaller than that of the standard laser array (~19°) and a single waveguide laser (~12°) [*Science*, Vol. 363, Issue 6427, pp. 623-626].

Results:

- High profile publication in journal *Science* demonstrating principles derived from supersymmetry with laser arrays
- Increased the power and efficiency of high power laser arrays by a factor of ~8 from a single element system
- Decreased diffraction in the far field which would otherwise limit the amount of power that can be delivered to a target

Way Ahead

With regard to the SUSY laser array, the output power as well as the radiance emerging from a single-mode SUSY laser array is expected to scale up with the number of elements involved. However, with additional elements one must pay greater attention to the role of nonlinearities that can lead to spatiotemporal effects. Further, improvements can be made by addressing fabrication imperfections. Additionally, the method introduced here can be used to design practical SUSY arrays at different wavelengths from the ultraviolet to the mid-infrared. Most excitingly, the result highlights that there are many more discoveries await application of SUSY elsewhere in optics and possibly beyond.

Quantum Information Science Program

Current Scientific Objectives

01

Extend the scientific understanding of multi-qubit and entangled quantum systems to ultimately enable advances in quantum computation and quantum networks that if successful, could enable beyond classical capabilities in computation, communication, and sensing

02

Establish the limits of the advantages of qubit-based quantum systems over classical systems for sensing and measurement that if successful could enable sensitivities physically unachievable by traditional, classical, systems for future applications such as resilient communications and sensor networks to protect the Soldier

03

Devise novel, primarily non cryptographic focused, algorithms to expand the application space of quantum information processing that if successful, could enable breakthroughs in fields ranging from machine learning, to optimization, to chemistry and materials science

Program Manager

Dr. Sara Gamble

Program Manager, Quantum Information Science
Physics Division
ARO Physical Sciences Directorate

Dr. Gamble completed her undergraduate studies at the University of Florida, receiving her B.S. in Physics in 2003. She trained as a physicist at Stanford University, receiving her Ph.D. in Applied Physics in 2010. She came to ARO in 2017 as the Program Manager for Quantum Information Science.

SUCCESS STORY

Light-Matter Entanglement Over 50 km of Optical Fiber

A U.S. Army research effort has established **light-matter entanglement through 50 km of optical fiber**, a procedure that could one day enable long distance quantum networks and make a quantum internet possible.

Challenge

A long standing roadblock for exploiting the advantages inherent in quantum information has been generating light-matter entanglement over any appreciable distance. Qubits, the fundamental unit of information in quantum information science (QIS), can be either physical (with mass) or photonic (light). A physical qubit has the advantage that we can exert more control over it. We can trap it in one place and more readily control its quantum state. A photonic qubit has the advantage that it can travel long distances while still maintaining its quantum state. Establishing light-matter entanglement and preserving it over appreciable distances is one of the first steps toward realizing distributed entanglement, which in turn will enable the advanced capabilities promised by quantum technologies such as tamper-evident communications, robust quantum networks, distributed computation, and quantum sensor arrays.

Action

ARO has supported basic research in quantum information science for over 20 years. This long standing and sustained effort has played a major role in the subsequent advances in quantum computing platforms, quantum sensing, quantum algorithms, and distributed quantum information. By 2015, basic research related to this latter thrust lead to the formulation of two programs aided in development by ARO PM Dr. T.R. Govindan, ARO Chief Scientist for physical sciences Dr. Peter Reynolds, and former ARO PM Dr. Henry Everitt. The first program was an Applied Research for Advancement of Priorities (ARAP) initiative supported by the Pentagon and targeted toward the development of quantum networks. The second program established a new center supported by CCDC ARL funds but composed of both extramural performers sourced from ARO's established 6.1 program and internal ARL research partners, highlighting the importance of ARO's 6.1 investments to ultimate transitions to work at ALC. This cooperative agreement based center focused on distributed entanglement and was named the "Center for Distributed Quantum Information" (CDQI). ARL program manager Dr. Grace Metcalfe took the lead in formally establishing and managing the CDQI and specifically challenged the community to establish a long distance multi-node quantum network. ARO QIS program manager Dr. Sara Gamble maintained an involvement in the CDQI program starting at its initiation, attending the kick-off and frequently talking with both the researchers on the extramural teams and the primary ARL scientists involved in the effort. Synergies between the research directions of CDQI and ARO's extramural program were strong and mutually beneficial, especially in areas exploring optimal schemes for creating and distributing entanglement.

This success supports these ARL Core Technical Competencies:

Network and Information Sciences

Computational Sciences

This success was made possible by the following ARO S&Es or Program Specialists:

- Dr. Sara Gamble, ARO Physics Division
- Dr. T. R. Govindan, NASA; ARO Physics Division

Upon Dr. Metcalfe's departure from ARL prior to the end of the five year CDQI program, official program management responsibilities for CDQI were moved from ARL SEDD to the ARO under the Quantum Information Science program managed by Dr. Gamble. Since taking over management in late FY18, Dr. Gamble has worked very closely with ARL scientist and Quantum Technology branch chief Dr. Fredrik Fatemi to ensure that the program continues to thrive. Programmatically, issues with disbursement, fifth year award extensions, and reporting were jointly worked through, and scientific results were shared at an annual review meeting in April 2019 attended by not only multiple ALC researchers, but also representatives from CCDC-Aviation and Missile Command, ARL Central, and AFOSR.

One of the cooperative agreements supported through CDQI is anchored at the University of Innsbruck, "Scalable Memory-Enhanced Ion-Trap Quantum Network" (SciNet). This team, led by Professor Tracy Northup, is composed of experts in multiple types of physical qubits: superconductors, trapped ions, and neutral atoms. The team also brought in experts in the types of physics and engineering necessary to work on the difficult problem of entangling these physical qubits with photonic qubits.

The major advance outlined in this story was achieved in the trapped ion system developed at Innsbruck by Dr. Ben Lanyon. Considerable engineering challenges needed to be overcome to achieve this result, such as the development of a reliable and controllable trapped ion system. One indispensable piece of enabling technology which was developed in the initial years of SciNet, however, is the periodically polled lithium-niobate (PPLN) crystal platform that converts the photon's wavelength into the telecom band while maintaining entanglement. By funding this multiyear effort, ARO PMs were able to focus research efforts on what are extremely challenging engineering tasks yet do not typically receive a high degree of attention from traditional engineering communities.

Result

In FY19, the University of Innsbruck team successfully created entanglement between a matter and photonic qubit, converted the wavelength of the photonic qubit to one amenable to transfer over standard telecom fiber, and transmitted the photonic qubit over 50 km of this fiber while preserving the entanglement. This incredibly impressive experimental success marks a major milestone in quantum information science and is the result of years of concerted effort across both the quantum information science and engineering communities.

The University of Innsbruck team works with $^{40}Ca+$ as its trapped ion qubit. This qubit interacts with light with a wavelength of 854 nm. In the experiment, the calcium ion is confined in a radio frequency (RF) linear Paul trap as well as an optical cavity. The RF Paul trap confines the ion via Coulomb interaction which is the interaction of the ion's electric charge with the field potential, and the optical cavity enhances photon collection. Entanglement is generated by driving atomic transitions with a pair of laser beams detuned far from the 845 nm transition wavelength, and the entanglement is encoded onto the polarization state of the photon.

The photon then undergoes a polarization preserving frequency conversion, which is a key engineering breakthrough in this system. The wavelength is converted to a new wavelength of 1550 nm using a technique called difference frequency generation

involving PPLN chips and a strong pump laser operating at 1902 nm. The photon is then coupled into a 50 km fiber spool. At the output of the spool a measurement is made on the photon and compared to a simultaneous measurement of the $^{40}Ca+$ ion.

Quantum state tomography, a common method of evaluating quantum processes, confirmed that the entanglement was preserved over the 50 km journey through the fiber. The detected generation rate of entanglement in this experiment is approximately once every second, but improvements on the detector side could push that number up by a factor of 20 with current technology. Additionally, the coherence time of the entangled state, which is the time the quantum state of the ion-photon pair remains preserved, is longer than 20 ms, making entanglement distribution over even greater distances possible. This result is a major milestone in networked quantum systems and promises to open the door to a wealth of new distributed quantum information studies.

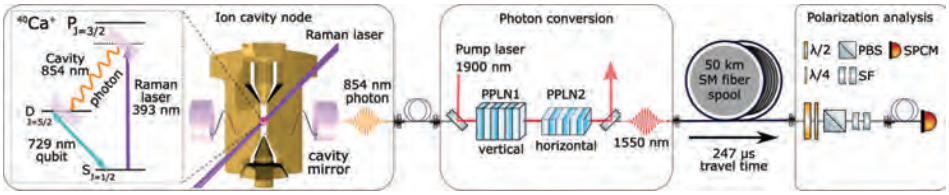


Figure 1: From left to right, a single atomic ion in a radio-frequency linear Paul trap and an optical cavity. A laser pulse triggers emission of an 854 nm photon into the cavity, which exits to the right. The photon is then wavelength-converted to 1550 nm and passes through a 50 km single-mode fiber spool and its quantum state is measured. (Krutyanskiy, et al., 2019; doi:10.1038/s41534-019-0186-3)

Way Ahead

Now that remote light-matter entanglement has been demonstrated, the next logical step is to establish matter-matter entanglement over significant distance. This will be done by replicating the ion-photon entanglement and then performing an entanglement operation on two photons which will in turn simultaneously entangle the two ions. This remote ion-ion entanglement, if successful, will be another key advance in establishing long distance quantum networks. One potential application of such networks is entangling quantum computing nodes, what some would call the nascent stages of a “quantum internet”. Though a quantum internet will not replace classical networks or exceed their speed of communication, it would provide unique capabilities not possible with classical computers and classical network connections. In the near term simple networks consisting of just a few qubits at each node could already enable powerful applications such as quantum enhanced distributed sensing, timekeeping, and cryptography.

This success supports these ARL Core Technical Competencies:

Network and Information Sciences

Computational Sciences

This success was made possible by the following ARO S&Es or Program Specialists:

- Dr. Sara Gamble, ARO Physics Division
- Dr. T. R. Govindan, NASA; ARO Physics Division

SUCCESS STORY

Quantum Logic Clock

This ARO funded research effort into a **trapped ion based quantum-logic clock** has resulted in the development of the highest precision time keeping device ever devised with a systematic uncertainty of less than a second every 33 billion years.

Challenge

Improving the performance of clocks has historically been one of the most vital efforts in our overall endeavor to ever enhance our abilities to navigate, locate, and explore. In modern times, atomic clocks have become the standard for precision timekeeping, and they are essential for the global positioning system (GPS). Additional precision can enable ever more complex autonomous navigation. Separately, atomic clocks enable record measurements of fundamental constants and enable us to achieve advanced sensing tasks. At the National Institute of Standards and Technology (NIST), researchers are continually pushing the boundaries of our timekeeping abilities, contributing to a cycle where better clocks lead to better measurement technology and better measurement technology leads to better clocks. The cycle constantly improves our ability to navigate, make precision measurements, and exert exquisite control.

Action

In 2010 ARO PM Dr. T. R. Govindan saw an opportunity emerging to explore novel ideas leveraging qubits to achieve new milestones in metrology. In response, he authored a MURI topic, “Multi Qubit Enhanced Sensing and Metrology” geared toward exploring these new possibilities. At the time, recent work in bulk atomic systems had demonstrated the extreme sensitivity of macroscopic quantum phenomena such as Bose-Einstein condensates’ sensitivity to magnetic fields. However, Dr. Govindan had the forethought to conjecture that one should be able to get enhanced sensitivity and better control with single or small nodes of qubits.

The MURI team ultimately selected consisted of top researchers from institutions including MIT, NIST, and Harvard. David Wineland had already begun working on quantum logic clocks at NIST at the time the MURI was initiated. As part of the MURI effort the research team proposed to utilize a single or multiple qubits as ancilla for enhanced readout and control. The team performed excellently on many fronts including quantum control, entangled atomic clock networks, magnetic sensing with Nitrogen vacancy centers, and beyond quantum limit sensing with squeezed states.

As the MURI progressed Dr. Govindan continued to fund a graduate student he had supported to complete his Ph.D. at MIT, Sam Brewer, for further post-doctoral work at NIST. There, he was able to work on the quantum logic clock with both Nobel Laureate Dr. David Wineland as well as Dr. David Leibrandt. Dr. Brewer and the ion storage team at NIST recently published their most recent result which is based partially on this work: the most precise atomic clock to date.

Result

In 1973, Hans Dehmelt proposed a frequency standard based on the extremely stable optical transitions of the elements Ti, B, Al, Ga, and In. The idea was to excite this

transition in a single ion, and the potential fractional frequency systematic uncertainty, a measure of merit for atomic clocks, was estimated at 10^{-18}. For reference, that extrapolates out to a variation of +\- 1 second every 33 billion years, or twice the age of the known universe. These experiment utilized Aluminum ions (Al^+), and while Al^+ is an exceptionally stable source of clock ticks, its properties are not easily manipulated or detected. So, logic operations with a partner magnesium ion (Mg^+) are used to cool the Al+ and to signal its ticks. The use of this Mg^+ control qubit enables researchers to maximally extract timing information from the Al^+ ion.

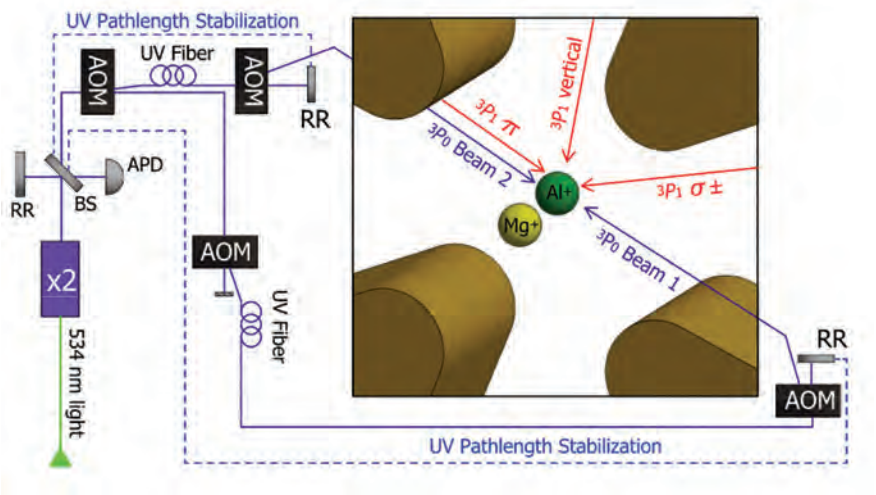


Figure 2: The Quantum-logic clock experimental setup. A laser is locked to an Al^+ transition ($\lambda \simeq$ 267 nm) by alternating the probe direction between two counter propagating laser beams (shown in violet). An enlarged view of the trapping region is shown on the right. (Brewer, et al., 2019; doi: 10.1103/PhysRevLett.123.033201)

Several technical advances enabled the improved performance of the logic clock, including a new ion trap design that reduced heat-induced ion motion, enabling operation near the desirable ground state, or lowest motional energy level. In addition, a lower frequency was used to operate the ion trap, reducing unwanted ion motion caused by the electric field used to trap the ions. Finally, improved quantum control via the Mg+ qubit has reduced the uncertainty of measurements of frequency shifts due to ion motion.

The fractional frequency uncertainty achieved in this work is $\Delta v/v=9.4\times10^{-19}$. This is the lowest systematic uncertainty reported for any clock to date and is in accordance with Dehmelt's original estimate. The clock is accurate enough to detect variation in time dilation effects due the earth's gravitational field on the order of a few cm. This experiment sets the bar for timekeeping and enables precision measurements. The constant improvement of atomic clocks will continue to provide increased navigational performance of GPS systems and enable better measurements of fundamental physical constants, and probe physics beyond the standard model.

Way Ahead

The NIST group is continuing to push the precision limits partially enabled by ARO's MURI investment even further in this quantum logic clock by improving the ion trap design, addressing uncertainty in the static differential polarizability, and reducing background gas pressure. Other efforts include utilizing entanglement to increase the number of atoms participating in a clock cycle, which would thereby reduce systematic uncertainty which

Results

- Record set for the lowest systematic uncertainty of any timekeeping device which extrapolates out to +\- 1 second every 33 billion years, or twice the age of the known universe.
- Result featured as an editor's suggestion in *Physical Review Letter* and promoted in many online science magazines.

scales as 1/√N. Efforts are also underway to take these atomic clocks out of the lab to enable enhanced Army capabilities related to precision position, navigation, and timing applications. Already atomic clocks, with albeit less precision, have been deployed in vibration and temperature stabilized trailers. Strides are being made on all fronts, and this result marks yet another record broken for precision in timekeeping.

Separately, Dr. Gamble is currently utilizing ARO's single investigator program to support Dr. Leibrandt to leverage and improve the quantum control techniques initially developed in relation to the clock work described here. This research aims to explore the limits of quantum control with molecular ion systems. This promising avenue may lead not only to advances in our fundamental grasp of physical constants and quantum chemistry, but also to the ability to control molecular ions as qubits for quantum information applications such as quantum computing.

The Army's Institute for Collaborative Biotechnologies (ICB)

Current Scientific Objectives

01

Focuses on studies to understand high-performance biological systems and create materials with resilient, robust functionality and performance for the future Soldier

02

Utilizes synergistic research utilizing academic investigators from the University of California - Santa Barbara (UCSB), the California Institute of Technology (Caltech), the Massachusetts Institute of Technology (MIT), and in collaboration with Army researchers and industry partners

Program Manager

Dr. James Burgess

Program Manager, Institute for Soldier Nanotechnologies and Institute for Collaborative Biotechnologies
ARO Physical Sciences Directorate

Dr. Burgess completed his undergraduate studies at Longwood University, receiving his Bachelor's degree in chemistry in 1992. He trained as a Bio-physical electrochemist at the Virginia Commonwealth University, receiving his Ph.D. in chemistry in 1997. He came to ARO in 2019 as the Program Manager for two UARCs: the Institute for Soldier Nanotechnologies and the Institute for Collaborative Biotechnologies.

SUCCESS STORY

ICB Microbial Fuel Cell Research Leads to Serendipitous Discovery of a New Class of Antimicrobial Compounds

Sustained ARO funding to discover the mechanisms of extracellular electron transfer in bioelectrochemical devices led to the **unexpected discovery of a new class of organic synthetic molecules** that are effective antibiotics for targeting multidrug-resistant pathogens.

Challenge

The emergence of multidrug-resistant (MDR) pathogens threatens a return of civilization to the pre-antimicrobial era. MDR pathogens are projected to kill 10 million people annually by 2050, and pose significant threats to Wounded Warriors. There are no known treatments for many MDR pathogens, nor are there promising candidates in the preclinical pipeline. Notably, there has not been a new class of broad-spectrum antimicrobials introduced for more than 50 years.

Sustained ARO funding for basic research on transmembrane electron transfer in microbial fuel cells through the Army's Institute for Collaborative Biotechnologies (ICB) University Affiliated Research Center (UARC) has led to the serendipitous discovery of a new class of antimicrobials, known as conjugated oligoelectrolytes (COEs), which have been shown to be efficacious against diverse MDR pathogens, including infections that are virtually untreatable with current antimicrobial agents. COEs are a class of small amphiphilic molecules that were designed to integrate into bacterial membranes and facilitate electron transfer for the development of microbial fuel cells. Their exciting potential as a new class of broad-spectrum antimicrobial compounds to aid the Warfighter has only recently been realized and will soon be further investigated with research support from both the ARO and the Walter Reed Army Institute of Research (WRAIR).

Action

In 2010, Dr. Robert Kokoska, who was then the Army's Institute for Collaborative Biotechnologies UARC Program Manager, invited Dr. Guillermo Bazan (UCSB) to submit a proposal "Transmembrane Electron Transfer for Energy Applications" for 2011 ICB UARC funding based upon preliminary results that had been found while working in close collaboration with Dr. James Sumner (ARL). The team discovered that it was possible to use conjugated oligoelectrolytes (COEs) to obtain a five-fold increase in the power production of yeast-based microbial fuel cells. These energy-generating devices were being considered for incorporation as the power source in unattended sensors and for wastewater remediation. At that time, it was not expected that this promising path of bioelectrochemical research would lead to new class of anti-microbial compounds.

The eventual discovery was enabled by ARO's UARC program managers Dr. Robert Kokoska and Dr. J. Aura Gimm, who supported and sustained an evolving and productive path of research in bioelectrochemistry, funded via the Army's ICB from 2011 to 2019. This

This success supports these ARL Core Technical Competencies:

Human Sciences

Protection Sciences

Materials and Manufacturing Sciences

This success was made possible by the following ARO S&Es or Program Specialists:

- Dr. Robert Kokoska, ARO Life Sciences Division
- Dr. James Burgess, ARO Life Sciences Division

collaborative basic program resulted in several publications that were jointly authored by researchers from the ARL and UCSB. It also resulted in United States Patent 8,614,021, "Agents for Enhanced Charge Transport Across Microbial Membranes," which was granted on December 24, 2013 to Guillermo C. Bazan and Logan E. Garner (UCSB) and James J. Sumner (ARL), and assigned to the United States of America as represented by the Secretary of the Army.

In June of 2019, Dr. Kokoska organized and chaired the Army's ICB Collaboration Working Group Meeting, where each of the Army's ICB project leaders briefed senior Army scientists, with the intent to obtain feedback and guidance from them as to where within the Army laboratory system they might find new scientific collaborators. It was during this meeting that Dr. Bazan presented several slides that provided details of this serendipitous discovery of the antimicrobial properties of COEs, and introduced his collaborator, Dr. Michael Mahan, who is a Professor of Microbiology at UCSB. Based on limited testing, Dr. Mahan had determined that particular COEs confer high efficacy and low cytotoxicity, are well tolerated in mice, exhibit low bacterial resistance and strong bactericidal activity, and can cure untreatable infections. Following the presentation, an SES-level scientist with the Army's Medical Research and Development Command volunteered to facilitate scientific discussions between Drs. Bazan and Mahan and the appropriate researchers at the Infectious Disease Center of the WRAIR. These discussions have resulted in a collaborative research and development agreement (CRADA) being negotiated between WRAIR and UCSB, which will allow further testing of the efficacy and toxicity of specific COEs at WRAIR during 2020.

Result

The discovery of conjugated oligoelectrolyte antimicrobial compounds derives from ARO funded studies on microbial electron transfer mechanisms. This was an innovative, vanguard research program to investigate the fundamentals of how it is possible to extract and inject electrons into microorganisms in order to obtain power or to promote chemical reactions. This basic research program has significant relevance to the Army, for on-site energy production for unattended sensors, waste water remediation, and modulation of biofilm properties and collective behavior. Through this research, the team found that it is possible to tune the collective selectivity and productivity of waste water biofilms to carry out specific chemical transformations. In collaboration with Army scientists, UCSB and the Army secured the intellectual property on ways to accelerate electron extraction from living microorganisms via use of conjugated oligoelectrolytes. It also resulted in multiple high impact scientific papers co-authored with Dr. James Sumner of ARL and Dr. Steve Harvey of CCDC Chemical Biological Center to demonstrate the evolution of wastewater bacteria into biofilms capable of converting waste into electricity.

This story recounts a serendipitous scientific discovery that was not foreseen by either the academic researchers or the ARO program managers and demonstrates that the future path of basic research programs cannot be predicted with certainty, and sometimes produce unexpected insights. The details regarding which specific conjugated oligoelectrolytes function against untreatable infections is currently protected under confidentiality agreements from public release; however, these details have been briefed to Army leadership.

Results

- Joint patent between Army and academic researchers on agents for enhanced charge transport across microbial membranes
- Multiple high impact scientific papers co-authored between Army and academic researchers
- Discovery of a new class of antimicrobial compounds that form the basis for a Collaborative Research and Development Agreement (CRADA) between academic and Army medical researchers
- Patented discovery: U.S. Patent 8,614,021 "Agents for Enhanced Charge Transport Across Microbial Membranes"

Way Ahead

CRADA is being established between the USCB, who will provide the novel COE antimicrobial compounds that have been discovered, and the WRAIR, who will perform both in vitro and in vivo testing and evaluation of the antimicrobial activity of the COEs against a variety of multi-drug resistant pathogens and also evaluate the toxicity of these compounds in animal models during 2020. Funding has been allocated within WRAIR for these tests and evaluations. The intent of this CRADA is to generate data that would provide sufficient preliminary data for support of a future grant submission (e.g., to the Congressionally Directed Medical Research Program).

In parallel, ARO's UARC Program Manager Dr. James Burgess is evaluating proposed research to explore conjugated oligoelectrolyte antibiotics. The goals of this new research initiative will be to (a) interface with Army collaborators at WRAIR so that COEs can be tested against a range of pathogens of relevance to the Army and its personnel, (b) determine the mechanism of drug action and resistance, and (c) examine how the structural modalities available for molecular design affect efficacy, toxicity, and drug resistance.

Interestingly, COEs have no structural relationship to any known antibiotic. These studies may therefore yield the first fundamentally new class of broad-spectrum antibiotics in fifty years. COE synthesis is relatively inexpensive and easy to scale-up compared to conventional antibiotics, with minimal decomposition even after years in solid or solution form without refrigeration.

The Army's Institute for Soldier Nanotechnologies (ISN)

Current Scientific Objectives

01

Focuses on studies for Nanotechnology-Enabled Enhanced Survivability for the Soldier

02

Synergistic research utilizing academic investigators from the Massachusetts Institute of Technology (MIT), in collaboration with Army researchers and industry partners

03

Integrates innovative Cutting-edge 6.1 & 6.2 Research Portfolio to Identify Revolutionary Opportunities

Program Manager

Dr. James Burgess

Program Manager, Institute for Soldier Nanotechnologies and Institute for Collaborative Biotechnologies
ARO Physical Sciences Directorate

Dr. Burgess completed his undergraduate studies at Longwood University, receiving his Bachelor's degree in chemistry in 1992. He trained as a Bio-physical electrochemist at the Virginia Commonwealth University, receiving his Ph.D. in chemistry in 1997. He came to ARO in 2019 as the Program Manager for two UARCs: the Institute for Soldier Nanotechnologies and the Institute for Collaborative Biotechnologies.

SUCCESS STORY

3D-Printed Shape-Shifting Soft Robots that can Crawl, Jump and Grab

This ARO initiative resulted in the **discovery of nanostructured functional links and a 3D-printing platform that can produce magnetically-actuated soft robotic structures** that may enable the creation of microscale robots to perform functions that are otherwise impossible for the Soldier to perform safely.

Challenge

The current generation of robots are rigid and cannot move dexterously in certain complex battlefield environments. Overcoming these limitations would require the discovery of new methods to integrate materials, metals, and polymers in flexible, relatively soft structures that are amenable to more flexible operations.

Action

ISN researchers developed a 3D-printing platform fitted with an electromagnet nozzle for use with a new type of 3D-printable ink infused with magnetic particles. This printing platform applies a magnetic field to the 3D printer's dispensing nozzle during its printing with an elastomer composite ink that contains ferromagnetic microparticles. The technique reorients the microparticles along the applied field and imparts a patterned magnetic polarity to the printed filaments. Using this approach, one can design structure and domain patterns, validate them with the model, and print them in order to actuate various functions. By programming the desired structure, domain, and magnetic field, one can print an intelligent machine such as a robot.

This success supports these ARL Core Technical Competencies:

Human Sciences

Protection Sciences

Materials and Manufacturing Sciences

This success was made possible by the following ARO S&Es or Program Specialists:

- Dr. Robert Kokoska, ARO Life Sciences Division
- Dr. James Burgess, ARO Life Sciences Division

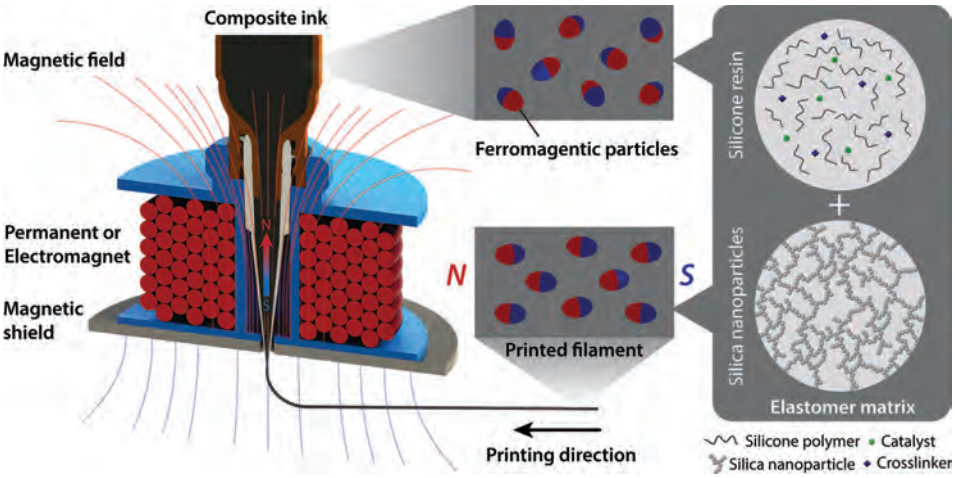


Figure 1: 3D-printing platform fitted with an electromagnet nozzle for use with a printable ink infused with magnetic particles.

Result

The ISN investigators developed a 3D-printing platform and a predictive model that enables both the modeling and design of complex magnetically actuated devices. The actuation speed and power density of the printed soft materials with programmed ferromagnetic domains are orders of magnitude greater than existing 3D-printed active materials.

This approach to soft robotics uses auxetic metamaterials that shrink in both the longitudinal and transverse directions when exposed to external magnetic actuation. This approach is different from the use of common materials which expand in directions orthogonal to the compressive load and different from typical auxetic materials that contract in directions perpendicular to the applied compressive mechanical force. Although others have fabricated magnetically activated materials to accomplish simple movements, this technique enables the modeling and the design of magnetically controlled device sections to perform complex Army relevant soft robotic tasks.

The method enables a set of previously inaccessible modes of transformation that can enable fast changes in 3D shapes such as a robot's limb. In one example using remote magnetic control, the researchers were able to demonstrate a metamaterial structure jumping forward 120 mm within 0.7 s due to the rapid release of the elastic and magnetic potential energy stored in the structure.

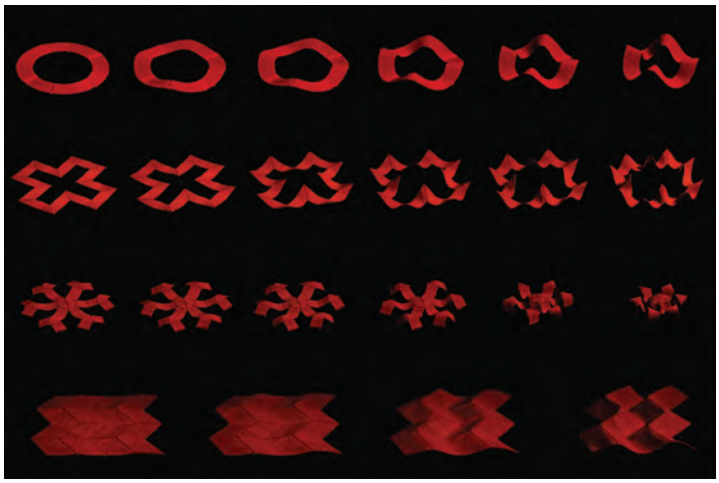


Figure 2: Time lapse photo for various designs of developed magnetic active material

Results

- Discovery of a new approach to model and design magnetically controlled devices to perform complex Army relevant soft robotic tasks.
- Discovery of a ferromagnetic soft continuum robotic approach that uses a robotic thread to slip through the brain's blood vessels in a step towards a minimally invasive robotic surgery technique for previously inaccessible lesions.
- *Nature* article titled "Printing ferromagnetic domains for untethered fast-transforming soft materials" (DOI/10.1038/s41586-018-0185-0)
- *Science Robotics* article titled "Ferromagnetic soft continuum robots" (DOI:10.1126/scirobotics.aax7329)
- ISN research featured on ARL Inside (https://arlinside.arl.army.mil/inside/news/articles/view.cfm?id=2185)

This discovery was featured in the Nature article titled "Printing ferromagnetic domains for untethered fast transforming soft materials" [https://doi.org/10.1038/s41586-018-0185-0], featured in ARL Inside, and featured at an ARL APG Seminar led by the ISN PI. A subsequent Science Robotics article titled "Ferromagnetic soft continuum robots" may open new pathways towards minimally invasive robotic surgery for previously inaccessible lesions (DOI:10.1126/scirobotics.aax7329).

This success was made possible through impactful teaming among ARL, the Army's ISN research team (Professor Xuanhe Zhao) and managed by the ARO ISN and ICB Program Manager, Dr. James Burgess.

Way Ahead

These findings could provide a step towards magnetic ink optimized to strengthen soft robotic functionality, new biomedical applications, or new on-demand flexible material systems for integration into Soldier systems enabling the Army's advanced manufacturing priorities.

The results may lead towards materials designed to provide future soft robotic capabilities. The 3D-printed robotic structures could squeeze into tight spaces like a crack in the wall of a cave, or jump over a trip wire or crawl under a vehicle, all complex Army-relevant functions impossible for humans to perform safely. The complex shape morphing structures could have great potential for the Army, because they may help create soft robots with pliable limbs similar to natural organisms.

SUCCESS STORY

Multimaterial Fiber Ink for 3D-Printed Devices that can Sense, Communicate and Store Energy

This ARO initiative resulted in the **discovery of structured multimaterial filaments for 3D printing of optical electronic components** (optoelectronics) that detect and control light that may lead to new devices for sensing, communication, or energy storage.

This success supports these ARL Core Technical Competencies:

Propulsion Sciences

Network and Information Sciences

Materials and Manufacturing Sciences

Challenge

The current generation of 3D printers that use single polymer filaments, experiences filament melting before the filament is extruded from the printer's nozzle. This creates a challenge when printing complex internal structures in a filament using different materials. The simultaneous 3D printing of disparate materials; metals, polymers and semiconductors with device quality interfaces and at high resolution remains a challenge.

Action

The ISN researchers developed a 3D printer with a special nozzle that is fed with a new kind of filament that has complex internal structures. These structured multimaterial filaments may enable future custom 3D functional devices not possible using existing approaches.

Result

Researchers at the ISN developed a new approach using a 3D printer fitted with a special nozzle, which unlike conventional printers, operates at a lower temperature and can rapidly pull a filament through the printer. In this approach, only the outer layer becomes partially molten while the interior stays cool and solid so any embedded electronic functions are unaffected. The approach uses a family of fibers to produce functional 3D devices that can sense, communicate or store energy. In one example the researchers fitted a model air plane with both light emitters and light detectors embedded in the material in an effort to continuously detect any microcracks as they begin to form.

Figure 3: Model air plane created using the ISN's new specialized 3D-printing system to contain both light emitters and light detectors embedded in the material, enabling the material to continuously detect any microcracks as they begin to form.

This discovery was featured in the Nature Communications article titled Structured multimaterial filaments for 3D printing of optoelectronics (DOI:10.1038/s41467-019-11986-0).

This success was made possible through impactful teaming among ARL, the Army's ISN research team (Professor Yoel Fink, and Professor John Joannopoulos, Director, ISN) and managed by the ARO ISN and ICB Program Manager, Dr. James Burgess.

Way Ahead

The ISN research team will continue collaborations with CCDC ARL, CCDC Soldier Center, the MIT Advanced Functional Fabric of America (AFFOA), and at the MIT Lincoln Laboratory Defense Fabric Discovery Center to explore how these findings can support the future Army's advanced manufacturing priorities.

This success was made possible by the following ARO S&Es or Program Specialists:

- Dr. Robert Kokoska, ARO Life Sciences Division
- Dr. James Burgess, ARO Life Sciences Division

Results

- Discovery of a new approach that uses a family of fibers to produce functional 3D devices that can sense, communicate or store energy.
- *Nature Communications* article titled "Structured multi material filaments for 3D printing of optoelectronics" (DOI: 10.1038/s41467-019-11986-0).

Chapter 04

Senior Scientist Showcase

The Army's senior scientist/technologist positions—known as STs—serve in general-officer level civilian positions advising leadership on scientific matters. This chapter provides a showcase of ARO senior scientists' initiatives and successes in FY19.

This background image is from "Designing Materials That Respond to their Environment" on page 70.

CHAPTER

04 Senior Scientist Showcase

Dr. Stephen J. Lee
Senior Scientist, Interdisciplinary, ARO

Dr. Lee completed his undergraduate studies at Millsaps College, receiving his B.S. in biology and chemistry in 1991. He trained as a physical organic chemist at the Emory University, receiving his Ph.D. in physical organic chemistry in 1996.

He came to ARO in 1998 as the Program Manager for what was then called the Organic and Inorganic Chemistry Program. In 2007, he became an Army corporate ST in the Executive Service spending time serving as the ARL Chief Scientist and the ARO Chief Scientist.

Dr. Stephen Lee is currently the ARO Senior Scientist for Interdisciplinary Sciences, which includes planning and developing the future vision of basic research for ARO while maintaining an active research program. His work at ARO includes basic research directed towards hazardous materials management, including studies in decontamination, detection, and protection.

Interdisciplinary Military Working Protection and Lethality

A revolutionary new hearing protection technology was developed to enhance the lethality and protection of the Military Working Dog (MWD), which has enhanced the operational window and capabilities of Special Operations Forces.

In 2019, a revolutionary new technology was developed to enhance the lethality and protection of the Military Working Dog (MWD). This hearing protection for the MWD has enhanced the operational window and capabilities of Special Operations Forces. Canis lupus familiaris (the domestic dog) is often overlooked for its long history of supporting military operations with the earliest recorded use being 600 BC against the Cimmerians. More modern use of MWDs has occurred from the mid-1600s through World War I and II into current operations. During this time canines have been used for a wide range of tactical and support operations by the United States Military. In October 2019, the importance of the MWDs in operations was best demonstrated by the highly publicized and important role of a special operations, multi-purpose canine in targeting ISIS leader al-Baghdadi. The MWD, Conan, conducted a key operational role of bringing the ISIS leader to justice by tracking down al-Baghdadi during the combat assault resulting in the ISIS leader's death. The dog acted as the only autonomous search system during this operation and many of the robotics research programs are working to replicate this already fielded capability. Generals Colin Powell, George Schwarzkopf, and David Petraeus, among others, have all recognized the profound impact of MWDs in operations supporting the Soldier.

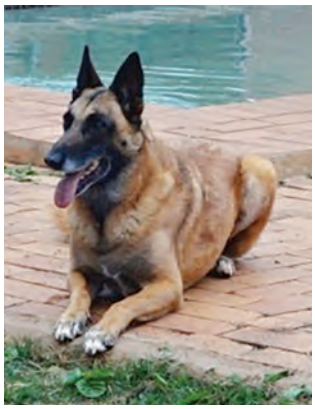


Figure 1: Testimonials of the MWD role in Army operations

"Technology, like the electronic frequency jammers used in Iraq to prevent bombs from being detonated by cell phones or TV remotes, has been successful, but the highest detection rates were still achieved using K-9 units and trained handlers."

LT. General Michael L. Oates, USA

"I often used war dogs in Vietnam in perilous areas where they quite literally saved many lives. There is no doubt that war dogs deserve to be recognized and honored for their service to our country and the National War Dog Team Monument is a most fitting tribute."

General H. Norman Schwarzkopf, USA

"War dogs have, indeed, served the nation well and saved many lives. Dogs continue to serve to protect Americans both in combat zones and in homeland security roles."

General Colin L. Powell, USA

"The capability they (Military Working Dogs) bring to the fight cannot be replicated by man or machine. By all measures of performance, their yield outperforms any asset we have in our inventory. Our Army (and military) would be remiss if we failed to invest more in this incredibly valuable resource."

General David H. Petraeus USA, 9 Feb, 2008

Historically, very little sustained science and technology research has been conducted for the MWD to support the Soldier, and that may come from a perception that they provide unpredictable low technology capabilities. In reality, the ability of the canine to work in a wide range of environments in combination with the Soldier and autonomous systems can greatly enhanced situational awareness of the individual Soldier in the future. MWDs address some of the primary needs of the Army with;

- Lethality – Tactical Canines
- Mobility – Detector Canines
- Survivability - Detector Canines
- Sustainability – Patrol Canines

Current military workings dogs are used by the U.S. Military for a variety of roles including tactical operations, patrol, detection and specialized search. The primary breeds are Labrador Retrievers, German Shepherds, and Belgium Malinois with an occasional specialized breed involved for unique missions.

At the heart of the MWD system is the handler and the canine. The vast majority of MWDs and handlers are trained at Lackland Air Force Base for the three Services. Over the years basic and applied research programs have attempted to build sniffers and sensors that will mimic the capability of the dog to detect chemicals but none have been shown to have near the sensitivity of the canine's nose. The combination of the dog's nose, mobility, versatility and intelligence as the platform for a "sensor" makes it very hard to replace as a unique capability. An example of a chemical sensor for explosives based on the dog's nose is the Fido NXT detector but by itself it doesn't replicate the entire capability of the canine with searching and the ability to follow the chemical trail to a source.

- Special Search Dog (SSD)
- Trace Explosive Detector Dog (TEDD)
- IED Detector Dog (IDD)
- Combat Tracker Dog (CDD)
- Patrol Dog (PD)
- Explosive Detector Dog (EDD)
- Multi-Purpose Canine (MPC)
- Drug Detector Dog (DDD)
- Patrol-Explosive Dog (P/EDD)
- Patrol-Drug Dog (P/DDD)

Figure 2. Breeds and different MWDs

However, the Fido sensor in certain instances can work longer and in more extreme environments than a MWD. Integration of the Fido XT explosives detector to robotic platforms makes one step towards creating a similar capability of canine but doesn't come close to the sensitivity and maneuverability of the MWD let alone addressing the relationship between the soldier and the MWD which makes it so successful.

Recently, the Canine Auditory Protection System (CAPS) has been developed under Army Research Office with Department Health Agency SBIR funding to Zeteo Tech, Inc. working with Dr. Pete "Skip" Scheifele of the University of Cincinnati. Dr. Scheifele is the leading animal audiology expert in the world today and works with MWD programs around the world to protect canine hearing.

High noise levels during training, transport, and operations can cause temporary and permanent hearing loss in working dogs. Even a short helicopter flight can affect a dogs hearing, resulting in impaired performance (i.e. inability to hear the handler's commands) and hinder the Soldier's mission.

Cumulative exposure can result in permanent hearing loss, reducing the dog's working life. The CAPS has been tested extensively with MWDs and Federal law enforcement working dogs. Dr. Scheifele has measured the hearing protection effectiveness of the CAPS during helicopter operations and has shown the dog's short-term hearing loss was significantly reduced.

The CAPS uses lightweight, high-quality acoustic absorption materials to block unwanted sounds. Unlike conventional hearing protection, the CAPS is constructed of flexible materials, easily conforming to the unique shape of a canine's head. This flexibility is key to ensuring proper sealing around the ear and maximum sound reduction. The "Snood" style headgear was designed to uniformly distribute the pressure required to hold the hearing protection in place, avoiding difficulties associated with straps.

Finally, at just over an inch thick, the CAPS low profile is not a hindrance when working in tight spaces and is compatible with other gear used by working dogs. This product for the MWD has transitioned from basic research in canine hearing through ARO programs to create a commercial product helping ensure Soldier lethality and protecting the MWD.

Ultimately, there are many opportunities for basic and applied research supporting the MWD. It is clear that, as a capability, the use of MWDs cannot be surpassed by any other system whether tactical or sensing at this time. There are many capabilities that can be leveraged for use by the MWD from the ongoing research within the Army and there are opportunities with the fielded MWD – Handler system to learn about how to integrate autonomous systems into the battlefield. The international community leads in the use of MWDs and likewise has a great deal of leadership in MWD science and technology, and the Army reaches out to the ongoing work in Europe. The MWD will continue to be utilized by the Army and research towards these needs above will help improve and enhance the capability of the MWD and the Soldier.

Figure 3. Fido NXT from FLIR.

Figure 4. Federal Law Enforcement Canine using the CAPS; **Figure 5.** Canine using CAPS in a Helicopter; **Figure 6.** CAPS is compatible with eye protection and other gear

Dr. Peter J. Reynolds
Senior Research Scientist, Physical Sciences, ARO

Dr. Reynolds has been a Senior Research Scientist at ARO since 2007. He started at ARO as a Program Manager in Atomic and Molecular Physics and became Physics Division Chief in 2004. Prior to joining ARO, Dr. Reynolds was a program officer at ONR from 1988-2003, a Staff Scientist at LBL from 1980-88, and an Assistant Research Professor at Boston University from 1979-80.

He has received the U.S. Presidential Rank Award as a Distinguished Senior Scientist in 2015, and is a Fellow of the American Physical Society. Dr. Reynolds obtained his Ph.D. in theoretical physics from MIT in 1979 and has an A.B. in physics from the University of California, Berkeley.

Co-Authored National Academy of Sciences AMO2020 Report

In 2018 Dr. Reynolds was selected by the National Academy of Sciences to become a member of one of its decadal review Committees. This Committee on the Decadal Assessment and Outlook on Atomic, Molecular, and Optical (AMO) Science, known as AMO2020 for short, was charged with undertaking a review of the AMO subfields of physics, considering issues such as the state of the AMO research community, international models for support and collaboration, and institutional and programmatic barriers.

He became a member of the AMO2020 Committee in the early summer of 2018. As a member of this Committee he participated in regular meetings and briefings, including from luminaries in the physics community. The Committee also made significant effort to solicit community input including via town hall meetings held at professional society meetings during 2018 and through a public website on which it received many white papers. Dr. Reynolds also actively provided his own input to the assessment, and is a co-author on the final National Academy report, which is to be published in early 2020.

The detailed task of the Committee was to survey the state of AMO science, and make recommendations on how the U.S. might better realize the full potential of the field. An important goal was to provide insights for not only the scientists comprising the AMO community, but for the federal Agencies involved with AMO, including the funding Agencies, and to provide recommendations to these Agencies and to Congress and other interested parts of the government.

The Committee was comprised of leaders from many different subfields within the AMO physics community, as well as prominent scientists from outside the field. The committee held five in-person meetings and numerous teleconferences among members to provide input, receive feedback, deliberate findings, and in the final months to collaborate on writing the report itself.

The report that resulted is structured around scientific grand challenges, with science goals, tool development, and research impact interleaved throughout the main science chapters. These summaries are intended as a guideline to identify the impacts of

The specific charges to the Committee were to:

- Review the field of AMO science as a whole, emphasize recent accomplishments, and identify new opportunities and compelling scientific questions.
- Use case studies in selected, non-prioritized fields in AMO science to describe the impact that AMO science has on other scientific fields, identify opportunities and challenges associated with pursuing research in these fields because of their interdisciplinary nature, and inform recommendations for addressing these challenges.

AMO science, now and in the coming decade, on emerging technologies and in meeting national needs. By highlighting a summary review of the field of AMO science as a whole, the report describes opportunities for scientific discoveries and new technological development. The insights sought from doing this study were with respect to finding opportunities to advance established and emerging areas of AMO through funding, education, and industrial partnerships, and to point out areas of anticipated growth, and to try to identify emerging areas.

The timing of this study and report overlaps with the currently increasing focus on quantum information science and technology (QIST) which has large overlap with AMO science. An entire chapter is devoted to it here. Not only does AMO help tackle some of the most fundamental questions related to quantum state engineering, entanglement generation and measurement, and controlled scaling of the number of qubits, but AMO also provides key enabling technologies and some of the most promising platforms that are critical for quantum science. In light of the strong national interest in QIST, as seen by the strong support for the NQI, it is clear that AMO will need to continue to play a large role both as basic science and for the role it plays in creating new opportunities for key enabling technologies for the progress of QIST.

The report contained a number of Findings and Recommendations, that are directed at the entire AMO research enterprise from scientists themselves, to government at various levels. Selected findings and recommendations are summarized here:

- Identify the impacts of AMO science, now and in the near future, on emerging technologies and in meeting national needs.
- Evaluate recent trends in investments in AMO research in the United States relative to similar research that is taking place internationally, and provide recommendations for either securing leadership in the United States for certain subfields of AMO science, where appropriate, or for enhancing collaboration and coordination of such research support, where appropriate.
- Identify future workforce, societal, and educational needs for AMO science.
- Make recommendations on how the U.S. research enterprise might realize the full potential of AMO science.

Finding: The historical strength of AMO has been in its core curiosity-driven AMO research programs, which have been the driving force behind many new scientific discoveries and innovative technologies, including the recent emergence of quantum technology.

Key Recommendation: It is vital that the U.S. government see curiosity-driven atomic, molecular, and optical science as a critical investment in our economic and national security interests and vigorously continue that investment to enable exploration of a diverse set of scientific ideas and approaches.

Finding: The development of quantum information science and technology is progressing rapidly, and, while the time is ripe to invest in quantum technology based on specific existing platforms, there is also a large and growing number of possible new systems and platforms one can exploit for construction of quantum machines.

Finding: The development of quantum technology is still at a very early stage, and the state of the art is evolving very rapidly. It is too soon to develop governmental standards; however, for the health of the field, the committee finds it is urgent for the research community to develop platform-independent metrics to measure quantum advantage and to characterize the true scientific impact of quantum advantage.

Key Recommendation: Basic research in science, engineering, and applications underlying both existing and emerging new platforms needs to be broadly supported, including research on techniques for cross-verification of quantum machines across different platforms for various applications. Specifically, the committee recommends that the National Science Foundation, Department of Energy, National Institute of Standards and Technology, and Department of Defense should provide coordinated

support for scientific development, engineering, and early applications of AMO-based quantum information systems.

Finding: Creative science carried out by single principal investigator (PI) groups is the heart of AMO science. The field does best building on these individual investigators, but it is entering a new phase where collaborations with flexible-size teams would enable exciting new discoveries.

Finding: The development of quantum technology is bringing new opportunities in sensing and precision measurement. However, nurturing these opportunities that impact other areas of science requires long-term investments that cross traditional disciplinary boundaries.

Finding: Experimental AMO science has become very expensive, and making the down payment to start up a new experimental program has become a deterrent for young AMO scientists being appointed as faculty in academia.

Finding: Strong theory-experimental collaboration has been important for maintaining the health of AMO science. However, the number of faculty positions in AMO theory has been limited.

Finding: There are existing successful portable funding models in the United States and Europe, such as the DOE early career, NIH-K99, and ERC grants, that could be used as models to assist faculty appointment and early career development. However, an aspect of the NIH-K99 that would not be appropriate for the U.S. academic physical science community is the level of research effort requirement that makes it incompatible with standard teaching expectations.

Finding: Departmental boundaries create barriers for young AMO-trained post-docs to move into related disciplines and departments, such as quantum information science, computer science, and electrical and mechanical engineering, where their AMO training could play key roles in advancing those fields.

Key Recommendation: Recognizing that the Department of Energy already deploys a portable fellowship grant model, the committee recommends that other AMO funding agencies should develop similar models that support the transition of AMO science theorists and experimentalists into faculty positions.

Finding: AMO science, like other physics disciplines, continues to have difficulty in attracting women and underrepresented minorities at all levels.

Finding: It is clear that education and workforce development in AMO is not keeping up with the demographic shifts in the nation, and that this is a lost opportunity.

Key Recommendation: The entire AMO science enterprise should find ways to tap into the growing national talent pool of women and underrepresented minorities. The committee therefore endorses the relevant recommendations in the National Academies reports Graduate STEM Education for the 21st Century and Expanding Underrepresented Minority Participation, for example.

Finding: Quantum technology cuts across scientific fields and technologies beyond AMO, and so encounters barriers with traditional funding mechanisms.

Finding: Traditional AMO training focuses on physics; however, the development of quantum technology requires reaching across both academic disciplines and industry to leverage the impact of AMO.

Finding: AMO technologies are not being transferred into other fields for use as rapidly as AMO science itself develops. It is increasingly important to let other fields become aware of AMO. The breakneck pace of AMO leads the committee to believe that other communities would benefit from knowing more about AMO.

Key Recommendation: The National Science Foundation, Department of Energy, National Institute of Standards and Technology, and Department of Defense should increase opportunities for translating atomic, molecular, and optical science advances to other fields by fostering collaboration with scientists and engineers from other disciplines through, for example, support of workshops and similar mechanisms for cross-disciplinary interactions.

Finding: The health of AMO science relies heavily on strong international collaborations. However, there exist a number of technical and regulatory impediments, including major differences in effort certification, IP ownership policies and conflict-of-interest rules, as well as unfunded external audit requirements and unreasonable currency exchange requirements, all of which make it difficult for U.S. universities to accept and administer grants from, for example, the EU. While the committee recognizes the significance of potential national security issues, there is great national benefit in having intellectual leaders visiting the United States. This benefit is at risk due to continuing significant issues affecting access to national research facilities and excessive visa delays for international students, collaborators, and speakers at conferences.

Finding: Mechanisms for co-funding research that is carried out with international collaboration fuels collective progress in AMO science.

The full report is expected to be published by the National Academy Press in early 2020. It is worth a look over by anyone interested in not only atomic, molecular, and optical sciences, but in any aspect of quantum information science and technology, or to see the enabling tools from AMO physics that impact fields as diverse as the hunt for exoplanets to medicine, and its strong interconnections to both old and emerging industry.

Army Innovations S&T workshop on Quantum Communication

In August 2019 the Army Senior Scientists (STs) held a set of Army Innovation S&T briefing for the Director of Research, Army Futures Command (AFC). These briefings were to assess Army priorities and technical gaps; to identify where the Army should lead, shape and watch; to influence future funding requirements in each of these focus areas; and to develop strategic plans for mid- to far-term Army research investments. The six focus topic areas were Hypersonics, Directed Energy, Quantum Communication, Cyber, Synthetic Biology, and Augmented/Virtual Reality. Each of the topic area briefings was followed by a small breakout session of under a dozen people of experts and interested parties.

Dr. Reynolds was the organizer and briefer for the quantum communication topic and lead for the breakout group. In his brief he started with an overview of the history of quantum mechanics, and how quantum information is a relatively new area, distinct from more traditional ("quantum 1.0") research. He went on to describe what the field of quantum information science (or "quantum 2.0") consists of, before specializing to a discussion of quantum communication and networking.

Advances in quantum information science, largely due to sustained investment by the DoD and Intelligence Community over the past 25 years, point to capabilities that are beyond those possible with classical systems. For the DoD broadly, and the Army specifically, these capabilities are about dominance in the collection, generation, processing, communication, and security of battle-space information. Battle-space information has become continual and enduring, and its volume is likely to be ever increasing in the foreseeable future.

All the Services have become aware of this, and have started their own investments in quantum information science and technologies (QIST). In a 2017 report to the Office of the Secretary of Defense (OSD), the Services jointly argue that "The field of quantum information science (QIS) has emerged as one of the most exciting areas of scientific research over the last three decades, exploiting the 'weirdness' of quantum mechanics to pursue computational capabilities and novel sensors with a speed and sensitivity impossible to achieve through purely classical means." They go on to say that "DoD technology strategy [should] intentionally mature selected QIS concepts that will deliver rugged, deployable, reliable capabilities in support of the challenging Command, Control, Communications, Computing, Cyber, Intelligence, Surveillance, and Reconnaissance (C5ISR) and Position, Navigation, and Timing (PNT) requirements emerging for this complex battlespace. Developing deployable quantum sensor technologies, including those that may exploit quantum entanglement, will provide unprecedented situational awareness and decision aids for manned and autonomous systems."

The beyond-classical capabilities of quantum information related technologies can be categorized in the areas of:

(a) Quantum sensors;

(b) Quantum computing and simulation; and

(c) Quantum communication and Quantum networking

Realization of these capabilities requires advances and solutions in many overlapping challenges. Moreover, the three above subtopics of QIS themselves overlap greatly; for example aspects of quantum computing are needed to achieve networking, while quantum sensors can be further enhanced on a quantum network.

After briefing this overview of quantum information, Dr. Reynolds focused on quantum communication and quantum networking. This can be viewed as research to enable beyond classical communications protocols and ways to distribute and use coherently various kinds of quantum states, e.g., for sensing.

The output of this workshop was a Report on quantum communication and networking that was requested by AFC, and has since been asked for by others for reference and planning, including most recently by members of the Networks Cross-Functional Team.

The Report focused first on Quantum networking as the overarching problem to solve, whose solution enables all of the Army required applications discussed in the Report. Quantum communication, in particular, critically needs the quantum network for secure multiparty communication protocols. However, distributing of quantum data across a set of nodes is critical for much more, including all the quantum enabled C5ISR applications mentioned here. Some of these applications are in communication, such as post-quantum authentication and security protocols, while others cut across other domains of quantum information.

It is important to note up front that quantum networks are not a replacement for classical networks (nor is quantum communication a replacement for classical communication; nor quantum computing a replacement for classical computing). A quantum network at its base consists of multi-node entanglement distribution (including the necessary protocols to do that); it includes small-scale quantum information processing necessary for error correction. Entanglement is intrinsic to many beyond-classical capabilities of quantum systems. Distributed entanglement enables the connectivity of spatially- and functionally-separated quantum systems, likely key to deployable and mobile quantum systems.

For quantum communication specifically, entanglement enables channel superactivation, as mentioned earlier. This can potentially enable one to communicate in a classically denied setting. Another aspect of communications on a quantum network is that it would eliminate the requirement for having trusted nodes along the way, which makes it quite distinct from quantum key distribution. Lastly, a host of security and authentication protocols are possible on a quantum network that do not exist in a point-to-point setting.

In the broader quantum information context, a quantum network enables both distributed and blind quantum computation; for assured PNT one gets distribution and synchronization of precise timing data; and for sensing considered generally one gets to coherently combine and manipulate sensor data. In other words, a quantum network, through its ability to distribute entanglement, a key quantum resource, enables enhanced as well as new Army capabilities in communication, information processing, and sensing.

The Report then moved on to a discussion of areas of QIS other than communication that nevertheless benefit from a quantum network include the following:

1. Precision navigation in GPS-denied environments
2. Precision timing for assured PNT
3. Optimization algorithms & simulation
4. Secure communications
5. Non-Inertial sub-shot-noise sensing (gravitational, magnetic, electric)

Dr. Bruce J. West
Senior Scientist, Mathematical Sciences, ARO

Dr. West graduated from the State University of New York (SUNY) at Buffalo with a B.A. in Physics in 1965. He graduated with a Ph.D. in nuclear physics from the University of Rochester in 1970, after which he was a post-doctoral researcher for two years before joining Physical Dynamics Inc. Beginning in 1976, he served as the Associate Director and later Director at the La Jolla Institute.

Before coming to ARO, Dr. West was professor of physics, University of North Texas, 1989 to 1999; chair of the Department of Physics, 1989 to 1993; and founding director of the Center for Nonlinear Science, 1994 to 1999. In 1992, he was elected a Fellow of the American Physical Society.

Dr. West joined ARO in 1999 as the Senior Scientist, Mathematical Sciences. He is a member of the American Physical Society, American Physiological Society, American Geophysical Union, American Association for the Advancement of Science, The New York Academy of Sciences, and he is an Adjunct Professor of Physics at Duke University (2000-present).

Sometimes a Good Idea

Dr. West decided to become a scientist because he was attracted to the ways in which experiment and theory were mutually supportive and how, with a proper model, he might be able to understand things that were still a mystery to others. Of course, he was 12 years old when he made that fanciful decision only shortly after reading the obituary of Albert Einstein. It was 1955 and he was graduating eighth grade, or he would be in the Spring.

Fast forward 60 years and beneath this thinning hair is that same boy with a memory of what had captured his imagination. What had been sparked was the desire to have a good idea. An idea that could change how people think about and understand the world. One way you can tell when an idea is good is by the unsolicited credit for its application received even before it is fully understood. This article presents his good idea, which he only began to appreciate this past year with the writing and publishing of *Empirical Paradox, Generating New Kinds of Knowledge [1]*.

As Mark Twain remarked [2]: "What gets us into trouble is not what we don't know. It's what we know for sure that just ain't so." In science the things that 'just ain't so' are theories that are wrong, but are believed by the vast majority of scientists. These are not merely errors of judgement, or sloppy mathematics, but well-argued mathematically-based theories that are supported by experiment – but are still wrong. This kind of contradiction he calls empirical paradox and probably requires some explanation.

In broad outline every discipline begins with elementary experiments, whose results are explained by simple models from which basic concepts are extracted. As a discipline matures the experiments become more sophisticated and these basic models are interwoven into ever more elaborate theories. Eventually, a point is reached where experiments probe the true complexity of a phenomenon and in order to explain the data, logical contradictions arise between two or more basic concepts. This is empirical paradox. Nature presents us with something that our logically constructed models tell us

[1] West B.J., K. Mahmoodi and P. Grigolini, Empirical Paradox, Complexity Thinking and Generating New Kinds of Knowledge, Cambridge Scholars, Cambridge, UK (2019).

[2] https://www.goodreads.com/quotes/738123-what-gets-us-into-trouble-is-not-what-we-don-t

cannot exist, but data tells us it does exist. Therefore the rigorously constructed discipline must reinvent itself, in whole or in part, to explain the contradictions implied by the new data, whose interpretation constitute the paradox. The resolution of the data-based paradox, which is a compromise between the conflicting partially true models, is achieved by changing how we think about the phenomenon, entailing a new kind of knowledge.

Dickens expressed the idea that paradox clearly exists within our everyday experiences. *A Tale of Two Cities* opens with the sentence [3]:

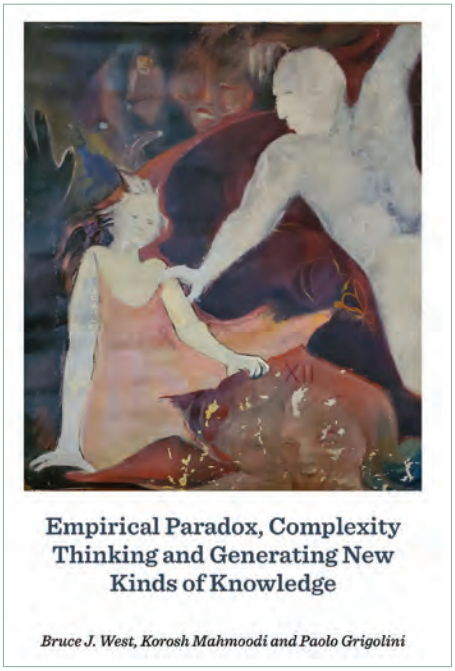
> *It was the best of times, it was the worst of times, it was the age of wisdom, it was the age of foolishness, it was the epoch of belief, it was the epoch of incredulity, it was the season of Light, it was the season of Darkness, it was the spring of hope, it was the winter of despair, we had everything before us, we had nothing before us, we were all going directly to Heaven, we were all going direct the other way.*

[3]Dickens C., A Tale of Two Cities, Centennial Edition, Heron Books; the final chapter was published in Dickens' circular, All the Year Round (1859).

Each of these binary oxymorons emphasizes a different aspect of complexity in European society at the time of the French Revolution. These paradoxical characteristics persist to be resolved in today's complex society just as they were in earlier societies. Their resolution produces different social orderings and the armies created to protect those societies reflect those new orderings, as well as, the strategies devised for their protection.

But no matter how strongly the words of the poet and author resonate with our experience, as scientists we require a different standard a truth. Our intuitive brain embraces these words and we understand them to convey a deep truth; a deep truth being a statement that along with its mirror image is true. At the same time our cognitive brain realizes that a statement and its negation cannot both be true and wants to reject the oxymoron out of hand. The implications of this ongoing conflict between the intuitive and cognitive brains in scientific research are the focus of these remarks and more importantly to the understanding of how science resolves empirical paradox. Scientists measure things. They examine the data from experiments and search for patterns. These patterns are identified as information about the phenomenon being measured. When intuitive understanding of these patterns reach a given level, cognitive models are constructed that can reproduce the individual motifs observed in the data. At this cognitive level the various models of phenomena thought to be connected to one another define what is loosely called a discipline. The models that make up a discipline are then joined into a theory. It is from such theory that knowledge flows.

The overhauling of theory to resolve contradiction occurs far more often in science than one might think. For example, contradiction resolution occupied most of the European scientific talent in physics during the second decade of the twentieth century, who pooled their collective intellect to answer the question: "Does light consist of waves, or does it consist of particles?" The answer should have been simple to obtain. Since physics is an experimental science, the procedure to obtain the answer should have been to examine the data and that should tell us if light is localized in space like a particle or is spatially distributed like a wave. The problem was that the data gave unambiguous patterns, some of which supported one interpretation, and some supported the other, depending on the measurement made. Consequently, the option of selecting one interpretation over the other was ruled out, since it would be necessary to discard half the data with either choice and that would be bad science. With either/or taken off the table, as in the case of light being either a particle or a wave, there only



Is another world war inevitable? The answer is a resounding "yes" if we continue to think in terms of "either/or" outcomes. Adversaries think in such terms, you either get what you want, or you do not. Can a different way of thinking produce a different outcome? This book shows that the consistency demanded by the linear, logical either/or thinking is disrupted by paradox, whose resolution forces a consequent decision: war or peace, with no middle ground. If this were the only way of thinking then a person would be either a protagonist or an antagonist, but a person can be both, either, or neither; this opens the door to novel solutions. This is "both/and" thinking, which the book shows can be achieved by a dynamic resolution of paradox. Thus, a basically selfish individual can also be a hero; a consequence of the complexity of being human.

Figure 1: Book cover: West B.J., K. Mahmoodi and P. Grigolini, Empirical Paradox, Complexity Thinking and Generating New Kinds of Knowledge, Cambridge Scholars, Cambridge, UK (2019)

remained one option that was consistent with data-based science, the both/and choice. Consequently, the final resolution of the nature of light paradox was accepting the notion of wave-particle duality, that is, abandoning the mutually exclusive concepts of particles and waves and accepting the empirical reality that light is both. This hypothesis required accepting the quantum as a physical parcel of light and exploring the implications of that hypothesis for other physical phenomena. Thus, quantum mechanics was born, and with it a complete change in the scientific view of the physical universe.

Dr. West attempted to organize the above ideas into a coherent whole within the pages of Empirical Paradox in a way that would be useful to the Army, without a great deal of success, when he had an epiphany. What he realized was that given: 1) the overwhelmingly complex nature of today's societies; 2) the U.S. Army is the most complex organization ever designed to perform a small number of functions; and 3) the information flow between two complex networks is determined by which is the more complex; that the Army leadership had to change the way it thinks about war. This is summarized on the back cover of the book (see Figure 1) [1]:

No doubt the formulation of the U.S. Army's protective strategy to integrate all the domains of warfare will, because of the fundamental complexity of the individual domains being integrated within a Multi-Domain Operation [4] (MDO), lead to internal contradictions. Any strategy of integration will require a new way of thinking; one that embraces contradictory alternatives, with the exclusionary either/or choice no longer being the "go-to" option it has been in the simpler societies of the past. But let us take a step back and examine the content of the MDO, where we find our adversaries have already implemented this kind of thinking.

[4]The U.S. Army in Multi-Domain Operations 2028, TRADOC Pamphlet 525-3-1, Dec. 2018

Under the umbrella of an expanding operational environment our adversaries have taken the distinct actions of "armed conflict" and "below armed conflict" and transitioned them from a historical either/or choice to a both/and choice. They have achieved this by blurring the distinction between the two actions, thereby allowing the two to exist simultaneously and enabling them to achieve their strategic objective without an armed conflict. This strategy, although attributed to our adversaries in the MDO document [3], had been openly discussed within our own national security community, under the concept of the "gray zone" conflict, for a number of years. Scientists paraphrase Brands' definition of the gray zone [5] to be activity that is coercive and aggressive in nature, and consciously designed to remain below the threshold of conventional military conflict. The intended goal is to reap gains normally associated with victory in open interstate war, but to achieve those gains without escalating to overt warfare, thereby avoiding the penalties and risks that such escalation might bring.

[5]Brands H., "Paradoxes of the Gray Zone", Foreign Policy Research Institute, E-notes

His purpose in detailing this particular aspect of MDO is to highlight the kind of strategy entailed by paradoxical thinking and which will be necessary to overcome an adversary who is already using it. A reader might conclude from this discussion that resolving the empirical paradox provides one with an alternative strategy, which it does. But it does much more than that.

This new kind of thinking arises by parsing existing knowledge into confrontational segments and resolving the resulting conflict [1]. Thus, producing a new kind of knowledge about how to prevail in conflict. This was done by Brands in his essay and was systematically explained by applying network theory to how we think where he [1] emphasized the importance of paradoxical thinking and the results obtained from its use in any one context are intended to clarify how it has already been applied.

Chapter 05

ARO Active MURIs

This chapter provides a brief summary of all ARO MURIs that were active in FY19, organized according to the year the MURI began. Each MURI is driving fundamental studies that will also impact one or more ARL Core Technical Competency, as indicated in the following table.

This background image is from "Materials with Extraordinary Spin/ Heat Coupling" on page 81.

CHAPTER

05 ARO Active MURIs

Index

ARO FY19 Success Stories with links to ARL Core Technical Competencies.

ARL Core Technical Competencies (CTCs)

The ARL technical strategy provides a comprehensive vision of the future technical landscape and is a critical component of its Research Management and Leadership Strategy. Key aspects of ARL's technical strategy are the seven Core Technical Competencies (CTCs) that guide the laboratory in identifying the scientific, technical, and analytical areas of vital importance to the Army of the future. These CTCs guide the laboratory in identifying and answering critical research questions in support of the Army's strategy for Multi-domain Operations and the required Army Functional Concepts. A brief summary of each CTC is provided in this section.

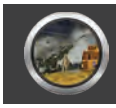
ARO's programs support each of the CTCs; however, as noted in Chapter 1, ARO's mission represents the most long-range Army view for changes in its technology, with system applications often 20-30 years away. ARO pursues a long-range investment strategy designed to maintain the Army's overmatch capability in the expanding range of present and future operational capabilities.

(M) Materials and Manufacturing Sciences

Research in this CTC drives the discovery and creation of superior materials and devices needed to enable lasting strategic land power dominance. The future Army will require materials with unprecedented properties rapidly manufactured, grown, synthesized, and produced cost-effectively to enable highly mobile, information reliant, lethal, and protected Army platforms. This technology enables the Army to execute real-time, point-of-need design and fabrication thereby increasing agility and logistical efficiency from the microscale to the infrastructure scale.

(C) Computational Sciences

This CTC focuses on advancing the fundamentals of predictive simulation sciences, data intensive sciences, computing sciences, and emerging computing architectures to transform the future of complex Army applications. Foundational research in artificial intelligence and machine learning will enable autonomous cross-domain maneuver warfighting concepts with intelligent agents that rapidly learn, adapt, and reason faster than the adversary to fight and win in contested, austere, and congested environments.



(B) Ballistics Sciences

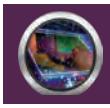
This CTC focuses on gaining a greater understanding and discovery of mechanisms and on generating concepts and emerging technologies that support kinetic lethality. Knowledge and concepts gained will lead to unprecedented enhancements in weapons range, precision, and lethality for the mounted and dismounted Soldier against a spectrum of manned and unmanned ground and aerial combat systems.

(H) Human Sciences

This CTC focuses on identifying, creating, and transitioning scientific discoveries and technological innovations underlying Human Behavior; Human Capabilities Enhancement; and Human-System Integration that are critical to the U.S. Army's future operational superiority. Foundational research in human agent teaming provides human agent teams with the capability to perform as well as Soldier teams but with greater team resilience, faster, more informed team decision making, and reduced numbers and risk to Soldiers.

(P1) Propulsion Sciences

This CTC focuses on gaining a greater fundamental understanding of advanced mobility and maneuver technologies that enable innovative vehicle configurations and subsystems architectures – critical to the future Army's movement, sustainment, and maneuverability. Foundational research in tactical unit energy independence enables energy-intelligent autonomous squad support systems that lighten the Soldier load, providing a more maneuverable, sustainable, and lethal force and intelligently monitor and distribute power on the move, reducing dismounted Soldiers' cognitive and physical load.



(N) Network and Information Sciences

This CTC focuses on gaining a greater understanding of emerging technology opportunities that support intelligent information systems that perform acquisition, analysis, reasoning, decision-making, collaborative communication, and assurance of information and knowledge. Understanding gained through these research efforts will lead to technological developments that make it possible to manage, utilize, and maintain trust in information flows and geospatial situational awareness within the battlespace.

(P2) Protection Sciences

This CTC focuses on gaining a greater understanding and discovery of mechanisms and generating concepts and emerging technologies that support protection systems that adapt to evolving threats, and the mechanisms of injury affecting the Warfighter. Foundational research in understanding and manipulating the physics of failure will lead to technologies that enable a broad array of resilient kinetic and non-kinetic protection systems and focuses on precise and accurate knowledge of materials/system failure for protection overmatch.

MURI Title	Pg #	M	C	B	H	P1	N	P2
New Start MURIs beginning in FY19								
How Sleep Clears Your Brain: Slow Waves, Glymphatic Waste Removal, And Synaptic Down-Selection	293				●			
Formal Foundations Of Algorithmic Matter And Emergent Computation	294	●	●				●	
Networked Palynology Models Of Pollen And Human Systems	294		●		●		●	
Near-Field Radiative Heat Transfer and Energy Conversion In Nanogaps of Nano- and Meta-Structured Materials	295	●	●				●	
Investigating Energy Efficiency, Information Processing and Control Architectures Of Microbial Community Interaction Networks	296		●				●	
Predicting and Controlling The Response Of Particulate Systems Through Grain-Scale Engineering	296		●			●		
Quantum State Control of Molecular Collision Dynamics	297		●			●		
Foundations of Decision Making With Behavioral and Computational Constraints	297				●		●	
New Start MURIs beginning in FY18								
Ab-Initio Solid-State Quantum Materials: Design, Production, and Characterization at the Atomic Scale	298	●					●	●
Multiscale Integration of Neural, Social, And Network Theory to Understand and Predict Transitions From Illness to Wellness	299				●			●
Multiscale Network Games of Collusion and Competition	300				●			●
New Materials from Dusty Plasmas	301	●						●
Quantum Control Based on Real-Time Environment Analysis by Spectator Qubits	302	●	●				●	
Science of Embodied Innovation, Learning and Control	303				●	●		
Stimuli-Responsive Control of Protein-Based Molecular Structure	303	●						●
Towards a Multiscale Theory on Coupled Human Mobility and Environmental Change	304				●			●
Active MURIs that began in FY17								
Abelian Bridge to Non-Abelian Anyons in Ultra-Cold Atoms and Graphene	305	●					●	●
Adaptive Self-assembled Systems	306	●						●
Data-Driven Operator Theoretic Schemes to Prediction, Inference, and Control of Systems	306			●		●	●	
Dissecting Microbiome-Gut-Brain Circuits for Microbial Modulation of Cognition in Response to Diet and Stress	307				●		●	●
Realizing Cyber Inception: Towards a Science of Personalized Deception for Cyber Defense	308		●				●	
Semantic Information Pursuit for Multimodal Data Analysis	309		●				●	
Active MURIs that began in FY16								
Closed-Loop Multisensory Brain-Computer Interface for Enhanced Decision Accuracy	309		●		●		●	
Defining Expertise by Discovering the Underlying Neural Mechanisms of Skill Learning	310		●		●			

MURI Title	Pg #	M	C	B	H	P1	N	P2
Discovering Hidden Phases with Electromagnetic Excitation	311	●					●	
Modular Quantum Systems	311		●				●	
Multi-modal Energy Flow at Atomically Engineered Interfaces	312			●		●	●	
Sequence-Defined Synthetic Polymers Enabled by Engineered Translation Machinery	313	●				●		●
Spin Textures and Dynamics Induced by Spin-Orbit Coupling	314	●					●	
Socio-Cultural Attitudinal Networks	315				●		●	●
Active MURIs that began in FY15								
Advanced 2D Organic Networks	315	●					●	
Emulating the Principles of Impulsive Biological Force Generation	315	●		●		●		
Engineering Exotic States of Light with Superconducting Circuits	316		●				●	
Fractional PDEs for Conservation Laws and Beyond: Theory, Numerics, and Applications	317		●					
Imaging and Control of Biological Transduction using Nitrogen Vacancy Diamond	318	●					●	●
Multi-Scale Responses in Organized Assemblies	319	●						●
Network Science of Teams	320				●		●	●
Noncommutativity in Interdependent Multimodal Data Analysis	320		●				●	
Active MURIs that began in FY14								
Attosecond Electron Dynamics	321			●		●		●
Force-activated Synthetic Biology	322	●						●
Innovation in Prokaryotic Evolution	322		●		●			●
Multiscale Mathematical Modeling and Design Realization of Novel 2D Functional Materials	323	●	●			●		
Multistep Catalysis	324	●				●		●
New Theoretical and Experimental Methods for Predicting Fundamental Mechanisms of Complex Chemical Processes	325	●				●		●
Ultracold Molecular Ion Reactions	326	●				●		●
Understanding the Skin Microbiome	326		●		●			●
Active MURIs that began in FY13								
Adversarial and Uncertain Reasoning for Adaptive Cyber Defense: Building the Scientific Foundation	327		●				●	●
Artificial Cells for Novel Synthetic Biology Chassis	328	●						●
Control of Complex Networks	328						●	
Materials with Extraordinary Spin/Heat Coupling	329	●				●		
Nanoscale Control, Computing, and Communication Far-from-Equilibrium	330		●			●		
Non-Equilibrium Many-Body Dynamics	330	●					●	
Theory and Experiment of Cocrystals: Principles, Synthesis and Properties	331	●		●		●		

Overview of Active ARO MURIs

The MURI program is a multi-agency DoD program that supports research teams whose efforts intersect more than one traditional scientific and engineering discipline. The unique goals of the MURI program are described in detail in Chapter 2. These projects constitute a significant portion of the basic research programs managed by ARO; therefore, all of ARO's active MURIs are described in this section.

Active MURIs that began in FY19

How Sleep Clears Your Brain: Slow Waves, Glymphatic Waste Removal, And Synaptic Down-Selection

This topic supports these ARL Core Technical Competencies:

Human Sciences

The MURI topic authors and co-managers of this project are Dr. Matthew Munson, Mechanical Sciences Division and Dr. Frederick Gregory, Life Sciences Division.

This MURI began in FY19 and was awarded to a team led by Dr. Nedergaard at University of Rochester. The goal of the MURI topic is to develop a framework describing the interplay of small- scale multiphase flows with biochemical and neurophysiological processes to quantitatively characterize glymphatic clearance dynamics and regulation mechanisms. This framework should account for disparate scales in both length and time, such that the reciprocal impact of cellular scale processes on system level regulatory phenomena (e.g. sleep) can be described and predicted. Additionally, strategies for exogenous manipulation of waste clearance to assess the impact on neurocognitive performance (e.g. alertness, learning, and memorization) should be explored.

The objective of this proposal is to examine the hypothesis that slow waves and the underlying ON/OFF bistability of thalamic and cortical neurons not only drive synaptic down-selection but also promote glymphatic flow by the coordinated movement of ions (Na^+, K^+, Cl^-) across the neuronal membranes during UP and DOWN states, which move from front to back and are detected as slow wave activity (SWA). The proposal seeks to: (1) demonstrate at the highest possible temporal and spatial resolution that glymphatic function, synaptic down-selection, and slow waves are linked; (2) characterize the underlying mechano-electro-chemical mechanisms that link these processes; and (3) determine whether facilitating these processes can increase the beneficial effects of sleep and improve neurocognitive performance.

Formal Foundations of Algorithmic Matter and Emergent Computation

The MURI topic authors and co-managers of this project are Dr. Samuel Stanton, Mechanical Sciences Division and Dr. Paul Baker, Physics Division.

This MURI began in FY19 and was awarded to a team led by Dr. Dana Randall, Georgia Institute of Technology. This MURI topic has two concurrent objectives: (1) Synthesize advances in nonequilibrium information physics with natural algorithms and decentralized control to identify principles governing how local algorithms, negative and positive feedback, fluctuation amplification, and the topology of information flow lead to unanticipated patterns and information processing in natural self-organizing systems. (2) Develop novel experimental systems to challenge and extend the theory and to additionally achieve directed self-organization. That is, demonstrate guided discovery of optimal information processing patterns or reconfigurable robustness to harmful emergent phenomena (e.g. failure modes) by actively biasing the environment or by manipulating the self-organization information-energy landscape.

This MURI focuses on systems that define algorithmic (active) matter: Ensembles of particles that interact locally leveraging their physical characteristics and their interaction with the environment, using limited computational resources, bounded communication, and bounded memory to achieve complex tasks.

The specific objectives of the proposed effort are to (1) predict physical and computational requirements for emergent computation, (2) determine what non-equilibrium characteristics cause these systems to evolve towards the desired emergent behavior, and (3) design efficient collective computational systems to achieve specific task-oriented goals.

This topic supports these ARL Core Technical Competencies:

- Network and Information Sciences
- Materials and Manufacturing Sciences
- Computational Sciences

Networked Palynology Models Of Pollen And Human Systems

The MURI topic authors and co-managers of this project are Dr. Micheline Strand, Life Sciences Division and Dr. Lisa Troyer, Life Sciences Division.

This MURI began in FY19 and was awarded to a team led by Dr. Anthony Grubesic, Arizona State University. The goal of this MURI topic is to develop both mathematical and computational modeling approaches that will transform our ability to model and predict the distribution of plant species and pollen across space and time. These advances will create a completely new capability; the ability to accurately model and predict species distribution, with human effects fully integrated.

The objective of the proposed research is for biologists, geographic information scientists and social scientists to work together to develop, instantiate, and validate networked palynology models of pollen and human systems in order to be able to exploit the geographic information embedded in pollen for forensic purposes.
The investigators will develop an open-source geocomputational toolbox based on next-generation species distribution models, which will locate forensic and other samples

This topic supports these ARL Core Technical Competencies:

- Human Sciences
- Network and Information Sciences
- Computational Sciences

that are geographically indeterminate based on inputs from pollen DNA metabarcoding. They will extend the use of standard DNA metabarcoding for identifying pollen samples, with a particular focus on quantification not just presence/absence. They will develop a rapid-deployment sampling framework for capturing airborne pollen and will also use pollinators as environmental samplers, particularly for low-abundance pollen. They will develop quantitative validation methods for determining the accuracy, precision and uncertainty of developed species distribution models and geocomputational models. Pollen samples including forensic, airborne, and pollinator from a variety of geographically known sources will be used. Finally, they will leverage their strengths in social network models and applications as well as mathematical optimization to enhance the inference and predictive elements of the proposed work in order to extend the model from single-location attribution to multi-location attribution.

Near-Field Radiative Heat Transfer and Energy Conversion in Nanogaps of Nano- and Meta-Structured Materials

The MURI topic authors and co-managers of this project are Dr. Chakrapani Varanasi, Materials Science Division and Dr. Marc Ulrich, Physics Division.

This MURI began in FY19 and was awarded to a team led by Dr. Sangi Reddy, University of Michigan - Ann Arbor. The goal of this MURI topic is to determine the mechanisms responsible for radiative heat transfer between the surfaces of nanomaterials and between meta-surfaces separated by nano-scale gap sizes in near-field and extreme near-field regimes and discover possible novel phenomena enabled by novel nano-materials /structures in these regimes.

The objective of this proposal is to understand the fundamental principles of novel near-field radiative heat transfer (NFRHT) phenomena such as NFRHT in Ångström-sized gaps (i.e. extreme NFRHT (eNFRHT)) and NFRHT between non-reciprocal, nanostructured 2D and phase change materials, as well as novel near-field energy conversion phenomena. The technical approach is based on a solid theoretical foundation and backed by sufficient computational studies. The proposed experimental platform to explore various NFRHT phenomena is proven and feasible. There is a series of novel materials and designs planned including dynamic control of NFRHT with phase-change materials, gate-tunable NFRHT, metasurfaces for spectral control and extreme NFRHT in nano-gaps. One novel and very exciting concept proposed by the team includes a persistent thermal current akin to the quantum Hall effect. The team has proposed a clever approach that should allow such counterintuitive persistent currents. Another strong component of the proposal is the incorporation of near-field energy conversion. By including thermophotovoltaics, into the NFRHT concepts, the team aims to advance the fundamental science and engineering of this aspect of energy conversion.

This success supports these ARL Core Technical Competencies:

Network and Information Sciences

Materials and Manufacturing Sciences

Computational Sciences

Investigating Energy Efficiency, Information Processing And Control Architectures Of Microbial Community Interaction Networks

The MURI topic authors and co-managers of this project are Dr. Robert Kokoska, Life Sciences Division and Dr. Derya Cansever, Network Science Division.

This MURI began in FY19 and was awarded to a team led by Dr. James Boedicker, University of Southern California. The goal of this MURI topic is to develop and validate a computational understanding of how information transfer arises within system architectures in biological communities across nature's evolutionary space and to identify universal scaling principles from those models that are common to these various community structures.

The objective of this MURI is to develop a comprehensive model of biological communication, by integrating four interconnected aspects of information flow within networks that span multiple scales of biological organization: 1) the connection between single-cell heterogeneity and decision-making within populations; 2) the optimization of information flow over multiple length and time scales; 3) the robustness and controllability of complex dynamic systems; 4) information exchange between multiple layers of biological organization and the scaling of communication architectures for unicellular organisms to networks of multicellular organisms.

This success supports these ARL Core Technical Competencies:

Network and Information Sciences

Computational Sciences

Predicting and Controlling the Response of Particulate Systems through Grain-Scale Engineering

The MURI topic authors and co-managers of this project are Dr. Joseph Myers, Mathematical Sciences Division and Dr. Julia Barzyk, Mechanical Sciences Division.

This MURI began in FY19 and was awarded to a team led by Dr. Jose Andrade, California Institute of Technology. The goal of this MURI topic is to enable efficient and accurate simulation of granular systems in nature and link particulate behavior across scales to enable efficient control algorithms within these systems.

This proposal will establish a framework to predict the continuum behavior of particulate systems by understanding and engineering a set of grain-scale features, termed here dynamic network attributes. The proposed work will develop the hypothesis that continuum behavior is encoded at the scale where neighboring grains interact. This proposal takes a radically different approach from the state-of-the art by directly embracing the interconnection between the different spatial scales that interact in granular assemblies: grain, mesoscale, continuum scale. The MURI builds on multiple areas of knowledge including Physics, Mechanics, Mathematics, and Engineering. The multidisciplinary approach affords the proposal the great advantage of transforming the state-of-the-knowledge across disciplinary boundaries that, historically, have been silos of

This success supports these ARL Core Technical Competencies:

Propulsion Sciences

Computational Sciences

specialized knowledge. Likewise, it will use and develop the most advanced experimental techniques (e.g., x-ray, force measurements) and connect these to continuum building blocks such as effective stress and constitutive models. Each of the areas is led by world-experts in the field. The project will also strike a balance between theoretical, experimental, and computational approaches covering more than 6 orders of magnitude.

Quantum State Control of Molecular Collision Dynamics

This success supports these ARL Core Technical Competencies:

Propulsion Sciences

Computational Sciences

The MURI topic authors and co-managers of this project are Dr. James Parker, Chemical Sciences Division and Dr. Paul Baker, Physics Division.

This MURI began in FY19 and was awarded to a team led by Dr. Arthur Suits, University of Missouri. The goal of this MURI topic is to prepare high densities of molecular species in selected vibrational, rotational, and angular momentum states and to study their reactive and non-reactive scattering dynamics in cold molecular beams.

The objective of the proposed research is the preparation of high densities of quantum states in molecular beams using techniques of quantum control and the study of quantum molecular collision dynamics as a function of the initially prepared state. Quantum degrees of freedom to be controlled in state preparation include translational, rotational, vibrational, and electronic. The research approach will draw on experimental and theoretical developments pioneered by the team members who hail from both chemistry and physics departments. Specifically, the team will pursue new coherent state preparation methods using lasers and molecular beams to generate molecules in perfectly-defined vibrationally excited initial states, then use these uniquely prepared reactants in novel scattering experiments. At the same time, state-of-the-art theoretical investigations of the interatomic forces and of the quantum scattering processes will be used to understand, model and interpret the experimental results. The effort will probe new aspects of molecular interactions and chemical reactivity under highly controlled conditions. The following thrust areas in the proposal relate to the various approaches to be taken: Stark-induced Adiabatic Raman Passage and Related Methods, Stimulated Emission Pumping, Photo Association and Direct Cooling, Machine Learning and Electronic Structure Theory, and Collision Dynamics.

Foundations of Decision Making with Behavioral and Computational Constraints

This success supports these ARL Core Technical Competencies:

Human Sciences

Network and Information Sciences

The MURI topic authors and co-managers of this project are Dr. Purush Iyer, Network Sciences Division and Dr. Edward Palazzolo, Network Sciences Division.

This MURI began in FY19 and was awarded to a team led by Dr. Ali Jadbabaie-Moghadam, Massachusetts Institute of Technology. The goal of this MURI topic is to create predictive models of information flow through (human) networks (with biases) through generalization of noncommutative probability theory and information theory.

The approach proposed by the Offeror is to interpret bounded rationality as the result of limited resources and ambiguity in language, among humans, rather than as one necessitating complicated mathematics to interpret humans. The team will use inspiration from successful use of resource-boundedness in Turing Machines to describe both structural and computational complexity, to derive a family of models between bounded and unbounded rationality. In doing so, the team will integrate both Cognitive Science and Computational Social Science perspectives to address problems in Decision Theory. Experiments by the cognitive scientists on the team would be used to validate the mathematical theories proposed.

The proposed approach is to approximate non-Bayesian reasoning using a form of Bayesian reasoning under structural and resource constraints, an idea borrowed from Complexity Theory in Theoretical Computer Science, starting with current work on explaining DeGroot style reasoning (a non-linear, non-bayesian) system as Bayesian reasoning under certain resource constraints. The proposed work will make use of ideas from non-linear utility, sampling, planning, distributed learning, computation complexity, etc, and is divided into three thrusts: (1) developing foundational models of individual decision-making under computational and cognitive constraints, aiming to build from principled and well-documented behavioral biases and deviations from rationality; (2) developing a theory of group decision making, along with a framework for analyzing decision-making models; and (3) computational and online experiments to test the theories from thrusts 1 and 2.

Active MURIs that began in FY18

Ab-Initio Solid-State Quantum Materials: Design, Production, and Characterization at the Atomic Scale

The MURI topic authors and co-managers of this project are Dr. Chakrapani Varanasi, Materials Science Division, and Drs. T.R. Govindan and Paul Baker, Physics Division.

This MURI began in FY18 and was awarded to a team led by Professor Dirk Englund at the Massachusetts Institute of Technology. The goal of this MURI is to develop novel solid state host materials with unique color centers exhibiting extraordinary quantum properties at room temperature (low spectral diffusion, long coherence times etc.), determine the composition processing defect property relationships governing these unique properties, and explore new concepts in quantum science (e.g. multi-photon states etc.) enabled by these new materials. In the long term, discoveries from this MURI may lead to several key quantum technologies, including single and entangled-photon emission, quantum sensors, and quantum memories.

Significant progress has been achieved in understanding and utilizing the quantum properties of optically addressable nitrogen-vacancy (N-V) color centers in diamond for quantum sensing and communication; however, further advances have been severely limited by difficulties in achieving exact placement of N-V centers, light collection due to the high refractive index of diamond, large scale integration, and low qubit yield. Superior solid-state host materials such as 3D wide bandgap semiconductors (e.g. SiC,

This success supports these ARL Core Technical Competencies:

Protection Sciences

Network and Information Sciences

Materials and Manufacturing Sciences

ZnO etc.) and recently discovered atomically thin two dimensional (2D) van der Waals materials (e.g. h-BN, WSe2). With varieties of optically addressable color centers (far beyond N-V centers) are very attractive alternatives to advance this science. In addition, these alternative materials could also offer new opportunities not yet accessible such as multi-photon states, interactions between color centers and non-linear quantum optics etc.

The MURI team will employ extensive expertise in ab-initio calculations, 2D materials fabrication and manipulation, 3D atomic imaging, and quantum spectroscopy to enable an integrated feedback loop of ab-initio design, fabrication, imaging, and characterization of quantum materials at the atomic scale. The team is also developing first-of-a-kind tools for reconstruction of 3D and 2D materials fully at the atomic scale, and develop revolutionary tools for nanometer-scale and even atomic scale fabrication of quantum emitter systems. Lastly, the team will develop revolutionary chip-integrated quantum devices, including for quantum error corrected memories, entanglement-assisted sensors, and superradiance/sub radiance control.

Multiscale Integration of Neural, Social, and Network Theory to Understand and Predict Transitions From Illness to Wellness

This success supports these ARL Core Technical Competencies:

Human Sciences

Protection Sciences

The MURI topic authors and co-managers of this project are Dr. Edward Palazzolo, Network Sciences Division, and Dr. Frederick Gregory, Life Sciences Division.

This MURI began in FY18 and was awarded to a team led by Professor Emily Falk at the University of Pennsylvania. The goal of this MURI is to identify and model the coevolutionary dynamics of neural, cognitive, and social networks as people transition between illness and wellness while engaged in rapid integration treatment modalities. In the long term, discoveries from this MURI may reveal the neural and social network mechanisms involved in the transition from illness to wellness, and identify specific mechanisms that can be efficiently targeted to identify and alter the trajectory of adverse behavior (e.g., substance abuse) that may impact an individual's or team's safety.

Network science advances in social network analytics and brain connectomics allow for greater understanding of network effects impacting mood and brain states. New mathematical and statistical models allow for unprecedented analysis of information dissemination and decision making. Recent research shows the impact of complex interactions between people's behavior and the route of messages through their social networks with respect to smoking behaviors, obesity, and the spread of happiness. Likewise, studies exploring mindfulness show measurable impact on human behavior as well as communication patterns between several brain regions. With greater understanding of the impact of social network connections (such as family, friends, healthcare teams, and weak ties) on the behavior of individuals embedded in society, attention must be turned to developing a foundational science to quantify how individuals' bodies and minds are impacted by such social forces and vice versa.

Neuroscience advances in mapping human neural activity can now be combined with social and cognitive network research to understand how people are connected to others and the causal impact of messages from their social network on changes in their brain states. These advances are relevant to understanding individuals who suffer from a variety of conditions such as PTSD, depression, anxiety disorder, substance abuse/addiction, and fibromyalgia/chronic pain.

This project is developing a multiscale model of intra-individual (i.e. neural, cognitive, physiological) and extra-individual (i.e. social) processes using an experimental manipulation of mindfulness and hypnosis, and characterizes interactions between baseline social network resources and regulatory strategy on dynamic neural responses and controllability, and downstream cognitive, physiological, and behavioral outcomes. The team will also experimentally perturb social network structure to further validate and refine the model.

Multiscale Network Games of Collusion and Competition

The MURI topic authors and co-managers of this project are Drs. Purush Iyer and Edward Palazzolo, Network Sciences Division.

This MURI began in FY18 and was awarded to a team led by Professor Mingyan Liu at the University of Michigan. The goal of this MURI is to create a new compositional Game Theory framework for characterizing dynamics of interaction between multi-genre networks that could potentially share members or have weak links. In the long term, discoveries from this MURI may lead to new methods to drive improved agility of DoD responses to a broad spectrum of real-world security risks, as risk heterogeneity is fundamentally tied to scale, spanning nation states and lone-wolf actors.

Advances in scalable algorithmic techniques have made Game Theory a practical tool in a number of security related applications, especially in the context of adversaries and defenders modeled in a 2-party game. In practical situations, however, there are social networks that underlie adversarial and defender groups, respectively, with potential weak links between members of opposing groups which are effectively used by both groups to infiltrate the other. Examples include the use of double-agents in infiltrating gangs and non-state adversarial groups, targeting of weak members in herd of deer, targeting of specific T-cells in tumors, etc. The dynamics of networks on networks is an ill understood problem, especially the use of weak links in strategic decisions. Furthermore, there are situations, such as in modeling adversarial groups embedded in an ally's host population, where the need to consider multi-party interactions at multiple scales becomes important. The host population while agreeing that the adversarial group is a threat to society is nevertheless sympathetic to the issues raised by the adversarial group. In such cases, an intuitive strategy might be to influence the sentiment of the masses while targeting individuals in the adversarial group with each success (or failure) of the defender resulting in a weakening (or emboldening, respectively) of the adversarial group. A meaningful mathematical analysis would require a multi-scale framework in which both coarse grained model (eg. of the host population) and fine grained model (of the social network of adversaries) need to be reasoned about.

This success supports these ARL Core Technical Competencies:

Human Sciences

Protection Sciences

This project is addressing the notion of abstraction and refinement in the context of network games, a class of n-party games where the network structure among the participants play a role in distributed strategies. The research is addressing inference and decision/control problems. The inference problems involve studies to identify multi-scale network structure from potentially incomplete observational data. The decision/control problems involve the design of effective control and intervention schemes at appropriate levels of the network in order to induce desirable individual as well as group behaviors.

New Materials from Dusty Plasmas

This success supports these ARL Core Technical Competencies:

Protection Sciences

Materials and Manufacturing Sciences

The MURI topic authors and co-managers of this project are Dr. Michael Bakas, Materials Science Division and Dr. James Parker, Chemical Sciences Division.

This MURI began in FY18 and was awarded to a team led by Professor Uwe Kortshagen at the University of Minnesota. The goal of this MURI is to elucidate and control plasma-material dynamics, concomitant with complementary novel consolidation strategies, to realize robust plasma-based synthesis of 3-dimensional (3D) free standing macrostructures via controlled consolidation of a wide range of discrete dust particles. In the long term, discoveries from this MURI may lead to directed energy applications, and advanced metamaterials with responsive properties for sensing and protection.

Research over the last decade has demonstrated that plasmas offer a means of levitating and manipulating “dust” particles of any material into controlled organized structures (i.e., plasma “crystals”) of up to tens of cm in size. Concurrently, magnetic plasma confinement chambers have shown abundant material accumulation and fast convective transport. This accumulation motivated advances in the understanding of plasma magnetohydrodynamics (MHD), in addition to accurate predictions of the spatial distribution of dust particles and their individual trajectories. These efforts provide the scientific basis to realize a new paradigm in custom material design: consolidation of 3D free-standing materials and structures from plasma “dust.” As plasmas can be created from any element and any material can be arranged in a plasma crystal, novel chemical reactions can be identified incorporating the free electrons, ions, and neutrals of a plasma to enhance manipulation and consolidation.

The MURI team is pursuing these studies at four highly interconnected levels: synthesis of particle building blocks, consolidation of these building blocks into macroscopic materials, materials design and characterization, and overarching theory and simulation. At the synthetic level, research will focus on advancing the state of the art from the current level of producing particles with homogeneous chemical composition of well-known phases to particle materials with nonequilibrium phases and composed of heterostructures. At the plasma consolidation level, the team will focus on controlling agglomeration to assemble macroscopic materials and elucidating the new physical mechanisms that will be encountered when incorporating dust crystals into free-standing macroscopic materials. Materials characterization will focus on establishing processing-structure-property relationships and on demonstrating new material design paradigms on testbed photonic materials.

Quantum Control Based on Real-Time Environment Analysis by Spectator Qubits

The MURI topic authors and co-managers of this project are Dr. T.R. Govindan, Physics Division and Dr. Samuel Stanton, Mechanical Sciences Division.

This MURI began in FY18 and was awarded to a team led by Professor Kenneth Brown at Duke University. The goals of this MURI are to discover and devise approaches in which new, sensing, "spectator" qubits enable real-time characterization and verification of classical environmental factors which, when uncontrolled, decohere qubits, and to develop optimal statistics and computer science based techniques for collecting and analyzing spectator qubit data. In the long term, discoveries from this MURI have broad applicability to all areas of quantum information science, which is of great interest to DoD for potential needs in logistics, optimization, and the quantum simulation of materials.

A multidisciplinary focus on qubit physics, materials, fabrication, and operation has resulted in orders of magnitude improvements in key qubit performance metrics. Concurrently, new computer science, statistics, and engineering based control techniques such as Hamiltonian parameter estimation, machine learning, and robust control of classical fields have enabled novel quantum control and feedback approaches. The time is opportune to expand the necessary multidisciplinary approach to a systems view of a complex quantum system operating in a classical environment by integrating the new control, feedback, and sensing concepts with qubit physics to provide the next order of magnitude improvement in qubit performance. Currently, in state-of-the-art, the qubit classical environment is rarely fully characterized during qubit operations in a qubit focused, rather than an integrated system focused, experiment.

Qubits often provide the most sensitive and precise measurements of the variability and noise in the classical environment in which they operate and, consequently, have recently been developed as high-performance sensing and metrology tools. Recent quantum sensing advances provide the opportunity for real-time control of the qubit classical environment via a novel combination of qubit sensing, statistics, machine learning, and control approaches. In the new paradigm, qubit sensor based characterization and verification of classical control fields conducted by a distinct set of "spectator" qubits located in the vicinity of the data qubits is visualized.

The MURI team is exploring this new paradigm by investigating the potential role of spectator qubits to quantify noise in quantum systems in real time and developing control strategies for high-performance operations that can be updated based on this information. The team will aim to characterize the noise using three methods: classical detectors, sensing with the data qubit, and real-time measurement of an integrated spectator qubit.

This success supports these ARL Core Technical Competencies:

Network and Information Sciences

Materials and Manufacturing Sciences

Computational Sciences

Science of Embodied Innovation, Learning and Control

This success supports these ARL Core Technical Competencies:

Propulsion Sciences

Human Sciences

The MURI topic author of this project is Dr. Samuel Stanton, Mechanical Sciences Division.

This MURI began in FY18 and was awarded to a team led by Professor Daniel Koditschek at the University of Pennsylvania. The goal of this MURI is to explore the emergence of embodied learning and control within natural and synthetic systems operating in uncertain and changing environments to develop a methodology that predicts statistical synchronization patterns between intrinsic nonlinear dynamics, sensing, and actuation to enable real-time model learning and adaptation. In the long term, discoveries from this MURI may lead to new paradigms to design and develop agile and dexterous autonomous systems capable of operating in any terrain and under battlefield conditions.

Progress in agile robotics has been limited by control methods reliant on optimization about linearized passive dynamics and nearly ideal sensing. A robot's mobility depends on its capacity to move energy from a store to its mass center along the right degrees of freedom at the right time by actuating appendages toward the periphery where it meets the environment. Because there is a premium on getting this work done quickly, power (the rate at which actuators can move Joules) is a first scarce resource. The information required to direct these outward flows appropriately must also be generated from some prior memory combined with feedback decisions made using real time streams. Moreover, since the purposes of mobility are inevitably linked to the robot's knowledge about the environment as well as the task, its ability to bring information from the periphery inward to the core at adequate rates inevitably presents a challenge simultaneous with and dual to its management of outward power flows.

A key focus of this research is to uncover the design of morphology, mainly the nature of limbs and body and their endowment with actuation and perceptual resources, to promote effective interaction between energy and information streams over contrasting scales of length and time. The project also aims to discover how to evolve, use and revise this endowment to achieve goal directed mobility and create new solutions to sensorimotor limitations and challenges represents the second focus.

Stimuli-Responsive Control of Protein-Based Molecular Structure

This success supports these ARL Core Technical Competencies:

Protection Sciences

Materials and Manufacturing Sciences

The MURI topic authors and co-managers of this project are Dr. Stephanie McElhinny, Life Sciences Division, and Dr. Dawanne Poree, Chemical Sciences Division.

This MURI began in FY18 and was awarded to a team led by Professor Milan Mrksich at Northwestern University. The goal of this MURI is to enable dynamic control over the motion of protein domains via incorporation of stimuli-responsive dynamic bonding chemistries (excluding disulfide/thiol linkages) to control protein function. In the long term, discoveries from this MURI may lead to engineered enzymes that provide a readily accessible supply of molecules that are currently difficult or impossible to produce or

protein biomaterials with tunable mechanical properties for broad applications from antibiotics to optical storage materials.

In biological systems, function is determined by structure. This structure-function relationship is particularly striking for proteins, where function is not solely determined by a static structure, but is also dependent on dynamic motions of subdomains within the folded protein. The most commonly observed domain motions are hinge and shear motions that occur in response to ligand binding, such as the hinge closure of hexokinase upon binding of glucose. To realize the full promise of engineered biological systems, mechanisms to exert dynamic control over protein structure are critical to enable regulation of protein activity.

Chemists have recently demonstrated incorporation of non-natural chemical functional groups into proteins that support synthetic bonding chemistries, including novel protecting groups that provide control over the accessibility of bonding moieties using applied external stimuli. Moreover, a variety of dynamic chemical switches have been developed for synthetic polymer systems in recent years, expanding the range of dynamic bonding chemistries that could be used for protein engineering. In recent years, a variety of dynamic bonding schemes have been introduced into synthetic polymer systems that enable triggered structural changes in response to applied stimuli, such as light, changes in pH, mechanical stress, and redox conditions. In these structurally dynamic polymers, macroscopic changes originate from a change in the polymer's molecular architecture through the controlled formation/breakage of bonds, providing a linkage between molecular structure and macroscopic properties that is not typically inherent in synthetic polymer systems. These dynamic chemical switches provide an opportunity to bring structural, and thus functional, control to protein biopolymers.

The MURI team is employing these biological and chemical principles to design reversible covalent chemistries that can be used to regulate the conformations of protein-based structures and combine experimental and computational approaches to design and demonstrate large-scale conformational changes in protein-based structures in response to an applied stimulus.

Towards a Multiscale Theory on Coupled Human Mobility and Environmental Change

The MURI topic authors and co-managers of this project are Dr. Lisa Troyer, Life Sciences Division, and Dr. Derya Cansever, Network Sciences Division.

This MURI began in FY18 and was awarded to a team led by Professor Rachata Muneepeerakul at the University of Florida – Gainesville. The goal of this MURI is to create a theory integrating environmental change, human social system dynamics, and the corresponding interdependencies, to create and validate predictive models that capture these dynamics to anticipate the trajectory of environmental change and human effects on these changes. In the long term, discoveries from this MURI may lead to new tools to advance situational awareness and facilitate operational decision-making, including the identification of emerging regions of potential conflict and risk.

This success supports these ARL Core Technical Competencies:

Human Sciences

Protection Sciences

Large-scale environmental changes such as floods, earthquakes, and droughts, can drive social mobility, which often precipitates new population migration patterns that in turn affect health, crime, and sociopolitical instability as humans relocate to access critical resources. However, the ability to model, theorize, and predict the interdependencies among environmental change and human social system dynamics remains a scientific challenge. Successful models of social-natural interdependence must account for the unique temporal/spatial scales of those systems, the factors determining action, and the natural and social constraints placed on those actions. These requirements pose substantial analytic challenges that no single discipline has been able to overcome.

This project is modeling population dynamics as movements of people over multilayer networks, each with interdependencies between natural environments and social institutions (e.g., governance structures, religious belief systems, kin networks). There will be four case studies that develop the modeling through natural disasters (e.g., hurricane), degrading economic systems (e.g., inflation), and two cases that integrate natural disasters and natural crises to capture secondary pushes that accelerate migration). Consequently, the project captures a range of effects across systems, including the ability to contrast sudden shocks and gradual degradations. An important feature of the modeling and testing approach is the use of Bayesian frameworks to assess the relative contributions of global sensitivity measures and expert opinion inputs on prediction of migration pathways.

Active MURIs that began in FY17

Abelian Bridge to Non-Abelian Anyons in Ultra-Cold Atoms and Graphene

This success supports these ARL Core Technical Competencies:

Protection Sciences

Network and Information Sciences

Materials and Manufacturing Sciences

The MURI topic authors and co-managers of this project are Drs. Paul Baker and Marc Ulrich, Physics Division, and Dr. Chakrapani Varanasi, Materials Science Division.

This MURI began in FY17 and was awarded to a team led by Professor Andrea Young at the University of California - Santa Barbara. The goal of this MURI is to unambiguously realize new systems exhibiting the physics of anyons and to verify their topological protection against decoherence.

The unparalleled potential capabilities of quantum sensors and quantum computers hinge upon finding systems that can be well controlled and robust against decoherence. Anyons are quasiparticles with fractional quantum statistics that can exist in low-dimensional systems and whose topological properties allow one to create quantum states that are protected from many sources of decoherence. The experimental evidence of the fractional quantum Hall effect (FQHE) was a landmark demonstration of topological order and fractional (anyonic) statistics in a two-dimensional electronic system. However, the fragility of the FQHE states, in which interesting anyons can exist, have prevented this approach from advancing despite decades of improvements in material quality. On the other hand, the recent experimental realization of Majorana modes by several groups provides an important scientific opportunity to explore these intriguing quasiparticles and provides a possible pathway to realize more general

anyonic systems. Advances in 2D materials, including topological surface states, new measurement capabilities, and recent theoretical progress in analyzing strongly correlated systems are rapidly advancing toward additional breakthroughs. This MURI effort will include studies of intrinsic anyons alongside extrinsic, synthetic approaches. The realization of these new robust states can pave the way for advances in universal decoherence free quantum sensors and computation as well as provide materials with currently unachievable properties that can be explored scientifically.

Adaptive Self-Assembled Systems

The MURI topic authors and co-managers of this project are Dr. Evan Runnerstrom (initially managed by Dr. John Prater), Materials Science Division, Dr. John Prater, Materials Science Division and Dr. Dawanne Poree, Chemical Sciences Division.

This MURI began in FY17 and was awarded to a team led by Professor Anna Balazs of the University of Pittsburgh. The goal of this effort is to develop experimental and theoretical approaches to integrate microscopic forms of self-organization with a scalable means of additive 3D fabrication.

Recent research related to the bottoms-up assembly of material has demonstrated the feasibility of using tailored short-range interactions to drive the assembly of functional clusters and macromolecular assemblies that are capable of performing basic functions such as catalysis, energy harvesting, color change and actuation. However, it is not currently possible to go beyond basic functionality and establish hierarchically ordered systems that display complex functional integration and dynamic system response. In particular, multifunctional structures with specifically targeted properties and robust feedback and control mechanisms that can embody aspects of emergent behavior and robust reconfiguration remain well beyond reach. This effort aims to establish the knowledge and expertise base needed to enable the design and directed assembly of nano-building blocks into complex, hierarchical 3D architectures capable of long-range control over multifunctional behavior and smart/dynamic responses using an additive 3D material assembly approach. The research is organized around three major thrusts: (1) assembly of microscale musculoskeletal frameworks, (2) transduction of energy to enable functionality, and (3) additive manufacturing of large-scale dynamic material systems. If successful, the research will enable the development of artificial “smart” materials and structures that exhibit tightly coupled capabilities for sensing environmental cues and then transducing energy to perform useful, situation-specific dynamic responses.

This success supports these ARL Core Technical Competencies:

Protection Sciences

Materials and Manufacturing Sciences

Data-Driven Operator Theoretic Schemes to Prediction, Inference, and Control of Systems

The MURI topic authors and co-managers of this project are Drs. Samuel Stanton and Matthew Munson, Mechanical Sciences Division.

This MURI began in FY17 and was awarded to a team led by Professor Igor Mezic of the University of California at Santa Barbara. The objective of this MURI is to develop a

This success supports these ARL Core Technical Competencies:

Propulsion Sciences

Ballistics Sciences

Network and Information Sciences

spectral decomposition theory that encompasses elements of ergodic theory, geometric theory of dynamical systems, and functional analysis via the spectral theory of linear infinite dimensional operators, control theory, machine learning for inference, prediction and uncertainty analysis.

The MURI team approach will be to study systems in which there exists a model (e.g. the Navier-Stokes equation for fluid flow) as well as systems with no model (e.g. data streaming either from physical sensors or unstructured data). In both cases the team will develop efficient methods to extract the correct descriptive variables via spectral properties of associated operators. The main theory topics to be pursued will expand the current reach of spectral expansion analysis: 1) Stability theory for general attractors; treatment of continuous spectrum; 2) Uncertainty analysis and spectral expansion theory of the Perron-Frobenius operator for observable evolution; 3) Extensions to inference, prediction and control; 4) Spectral expansions for finite-time analysis; 5) Non-smooth systems. The main numerical analysis topics to be pursued will expand the current reach of spectral expansion analysis: 1) Proofs of convergence of finite-dimensional approximations to spectral objects of the infinite-dimensional Koopman and Perron-Frobenius operators; 2) Algorithms for finite-time analysis in nonautonomous and control systems; 3) Algorithms for extraction of finite-dimensional models from data for inference, prediction and control; 4) Rigorous utilization of machine learning algorithms in spectral expansion theory; 5) Utilization of spectral expansion theory for development of next-generation, real time computational tools for complex physics; applications to vortex dynamics. Finally, the team will investigate experimental and data analysis topics to expand the current reach of spectral expansion analysis: 1) Network monitoring problems arising in cybersecurity; 2) Experiments in locomotion for a class of hybrid oscillators; 3) Experiments on finite-time vortex stability; 4) Experiments on one of the most vexing continuous spectrum problems - turbulence in fluid-structure interactions leading to large deformations. All of these areas span DoD interests such as helicopter dynamics, robotics and cybersecurity. These developments in this MURI will lead to a massive changes in design, data inference, and control of systems possessing a very broad set of nonlinear features.

Dissecting Microbiome-Gut-Brain Circuits for Microbial Modulation of Cognition in Response to Diet and Stress

This success supports these ARL Core Technical Competencies:

Human Sciences

Protection Sciences

Network and Information Sciences

The MURI topic authors and co-managers of this project are Drs. Frederick Gregory and Robert Kokoska, Life Sciences Division.

This MURI began in FY17 and was awarded to a team led by Professor Elaine Hsiao at the University of California - Los Angeles. The objective of this MURI effort is to investigate how the community of microorganisms naturally residing in the human gut (i.e., the gut microbiome) alters cognitive performance in response to nutritional and physical stress.

Recent studies from several laboratories reveal that the responses of the human microbiome, and specifically the gut microbiome, responds to environmental factors (e.g., diet and stress) in a way that modulates host brain activity and behavior.[1-3] The objective

of this MURI is to uncover gut microbiome influence on host neurobiology, develop a layered cellular and systems-level model and theory of cognitive and behavioral control by commensal gut microorganisms and extract integrated neural, endocrine, immune and gut microbial interaction principles governing nutrition and physical stress response.

This MURI, if successful, will provide sophisticated predictive tools available to the academic community and DoD upon which more comprehensive biological studies could be performed to more completely understand causative effects throughout this complex networked system. These models have the potential to far exceed current state-of-the-art by offering a currently unavailable analytical framework for future discoveries. The long term potential applications could be the rational design of probiotic regimens to ameliorate symptoms of anxiety-like disorders including PTSD, methods to manipulate the gut microbiome to affect human performance without the need for genetically engineering the human host. Outcomes of this MURI would also direct whole-force recommendations to the Army Surgeon General's Performance Triad and Brain Health Campaigns.

[1]*Magnusson KR, Hauck L, Jeffrey BM, Elias V, Humphrey A, Nath R, Perrone A, Bermudez LE. (2015). Relationships between diet-related changes in the gut microbiome and cognitive flexibility. Neuroscience. 300:128-40.*

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[3]*Bravo JA, Forsythe P, Chew MV, Escaravage E, Savignac HM, Dinan TG, Bienenstock J, Cryan JF. (2011). Ingestion of Lactobacillus strain regulates emotional behavior and central GABA receptor expression in a mouse via the vagus nerve. Proc Natl Acad Sci U S A. 108:16050-5.*

Realizing Cyber Inception: Towards a Science of Personalized Deception for Cyber Defense

The MURI topic authors and co-managers of this project are Dr. Cliff Wang, Computing Sciences Division and Dr. Lisa Troyer, Life Sciences Division.

This MURI began in FY17 and was awarded to a team led by Professor Milind Tambe at the University of Southern California. The goal of this MURI research is to gain scientific understandings to significantly advance the state of art in learning and modeling of adversarial mental states and decision processes, to create metrics quantifying information effectiveness in driving cognitive state change under the deception context, and to build an integrated framework of deception composition and projection methods to successfully manipulate adversaries' mental state and decision-making process to our advantages.

The research focuses on an innovative and comprehensive study of adaptive cognitive modeling, cyber deceptive game theory, and deception and monitoring systems that. The effort consists of three major thrusts: 1) Deception and Monitoring Systems: Ultimately deceptive strategies developed by higher-level reasoning about the attacker must be realized in a system, in such a way that the deceptions are convincing and their effects on the attacker can be effectively monitored. 2) Cyber Deceptive Game Theory: Game theory provides a mathematical framework for modeling the interactions between defenders and attackers in cybersecurity, which is an important foundation for developing a science of security. Developing game-theoretic models and algorithms for cybersecurity will allow richer modeling of adversarial interactions, a deeper understanding of deception and information manipulation tactics, and more effective response strategies. 3) Cognitive Modeling: Cognitive models provide a computational representation of human cognitive processes, their detailed mechanisms and limitations, and the knowledge upon which they operate. By taking advantage of human bounded rational decision behavior, where humans make decisions according to the constraints on the environment of their own cognitive limitation, the team will build a personalized model of adversary behavior.

This success supports these ARL Core Technical Competencies:

Network and Information Sciences

Computational Sciences

Semantic Information Pursuit for Multimodal Data Analysis

This success supports these ARL Core Technical Competencies:

Network and Information Sciences

Computational Sciences

The MURI topic manager of this project is Dr. Cliff Wang (initially managed by Dr. Liyi Dai)Computing Sciences Division.

This MURI began in FY17 and was awarded to a team led by Professor Rene Vidal of Johns Hopkins University. The goal of this research is to establish the theoretical foundation for context and principles of information physics for data analysis that provide an analytical framework and computation algorithms for the characterization, analysis and understanding of information content in multimodal data.

The proposed information-theoretic framework for characterizing information content in multimodal data combines principles from information physics with probabilistic models that capture rich semantic and contextual relationships between data modalities and tasks. These information measures will be used to develop novel statistical methods for deriving minimal sufficient representations of multimodal data that are invariant to some nuisance factors as well as novel domain adaptation techniques that mitigate the impact of data transformations on information content by finding optimal data transformations. The computation of such optimal representations and transformations for classification and perception tasks will require solving nonconvex optimization problems for which novel optimization algorithms with provable guarantees of convergence and global optimality will be developed. The uncertainty of such information representations derived from multimodal data will be characterized via novel statistical sampling methods that are broadly applicable to various representation learning problems. The information representations obtained from multiple modalities will be integrated by using a novel information theoretic approach to multi-modal data analysis called information pursuit, which uses a Bayesian model of the scene to determine what evidence to acquire from multiple data modalities, scales and locations, and to coherently integrate this evidence. The proposed methods will be evaluated in various complex multimodal datasets, including text, images, video, cellphone data, and body-worn cameras.

Active MURI's that began in FY16

Closed-Loop Multisensory Brain-Computer Interface for Enhanced Decision Accuracy

This success supports these ARL Core Technical Competencies:

Human Sciences

Network and Information Sciences

Computational Sciences

The MURI topic authors and co-managers of this project are Dr. Cliff Wang (initially managed by Dr. Liyi Dai), Computing Sciences Division and Dr. Frederick Gregory, Life Sciences Division.

This MURI began in FY16 and was awarded to a team led by Professor Maryam Shanechi at the University of Southern California. The goal of this research is to create new methodologies for modeling multimodal neural activity underlying multisensory processing and decision making, and to use those methodologies to design closed-loop adaptive algorithms for optimized exploitation of multisensory data for brain-computer communication.

This research effort will contribute to the development of a new closed-loop brain-computer interface (BCI) framework for enhancing decision accuracy. The framework will collect multimodal neural, physiological, and behavioral data, decode mental states such as attention orientation and situational awareness, and use the decoded states as feedback to adaptively change the multisensory cues provided to the subject, thus closing the loop. To realize such a framework, the effort will make fundamental advances on four fronts, constituting four research thrusts: (1) modeling multisensory integration, attention, and decision making, and the associated neural mechanisms; (2) machine-learning algorithms for high-dimensional multimodal data fusion; (3) adaptive tracking of the neural and behavioral models during online operation of the BCI; and (4) adaptive BCI control of multisensory cues for optimized performance. Complementary experiments with rodents, monkeys, and humans will be conducted to collect multimodal data to study and model multisensory integration, attention, and decision making, and to prototype a BCI for enhanced decision accuracy. The modeling efforts will span Bayesian inference, stochastic control, adaptive signal processing, and machine learning to develop: (1) novel Bayesian and control-theoretic models of the brain mechanisms; (2) new stochastic models of multimodal data and adaptive inference algorithms for this data; and (3) novel adaptive stochastic controllers of multisensory cues based on the feedback of users' cognitive state.

Defining Expertise by Discovering the Underlying Neural Mechanisms of Skill Learning

The MURI topic authors and co-managers of this project are Dr. Frederick Gregory, Life Sciences Division and Dr. Virginia Pasour, Mathematical Sciences Division.

This MURI began in FY16 and was awarded to a team led by Professor Scott Grafton at the University of California – Santa Barbara. The goal of this MURI is to uncover the temporal dynamics of neural substrates and cognitive processes engaged during skill learning and generate a definition of expertise based on the underlying neurocognitive computational advantages generated through learning.

Neuroscience, social psychology and education are providing insights into neural and cognitive processes involved during skill learning which show structural and functional differences in multiple brain regions when compared between 'experts' and 'novices'. Typically, these comparisons involved a novice time point and an expert time point because of the difficulty measuring intracranial brain activity over the course of skill learning. Novel materials now enable long-term implantation of high density neural recording devices in humans and animal models. Emerging engineering breakthroughs enable spike and local field potential recording from multiple neuroanatomical sites in the brain simultaneously. However, a major analytical barrier prevents easily linking this high density data with data acquired through existing non-invasive electrophysiology techniques and other tools for determining structure-function relationships like magnetic resonance imaging.

The objective of this research is to develop tools and techniques that can both predict and explain from a neurobiological perspective, why there are differences among

This success supports these ARL Core Technical Competencies:

Human Sciences

Computational Sciences

individuals in their ability to develop expertise. The future force demands expert soldier performance across many tasks. In the long term, this basic research effort will provide a critical foundation for developing training methods based on computational and network neuroscience that are grounded in neurophysiology and neuroanatomy.

Discovering Hidden Phases with Electromagnetic Excitation

This success supports these ARL Core Technical Competencies:

Network and Information Sciences

Materials and Manufacturing Sciences

The MURI topic authors and co-managers of this project are Dr. Marc Ulrich, Physics Division and Dr. Chakrapani Varanasi, Materials Sciences Division.

This MURI began in FY16 and was awarded to a team led by Professor David Hsieh at the California Institute of Technology. The goal of this project is to create new electronic states of matter that are unobtainable through conventional solid-state synthesis, which in the long term may lead to enhancements of electronic, optical, magnetic and thermal material properties that would lay a foundation for future technology in many areas.

Nascent research has demonstrated unique phases that are not adiabatically accessible from the known phase diagram. Recent discoveries have involved photo-excitation of a material with an ultra-short pulse which non-adiabatically induces a phase distinct from that existing elsewhere on the ground state phase diagram. Examples include a non-equilibrium superconducting state in a BCS superconductor, a ferromagnetic state in an antiferromagnetic oxide, and a unique metallic state in a thin film of a dichalcogenide. The team is attempting to employ excitations across the entire electromagnetic (EM) spectrum, including with extremely high pulsed fields, to design, realize, and manipulate new phases and responses in strongly correlated materials. Specifically, the team will focus on realizing new correlated states via the following approaches, (1) EM stimulated, bond selective, tuning of charge hopping parameters, (2) direct EM modification of magnetic exchange, order, and frustration, (3) continuous EM control of dimensionality and hybridization, and (4) EM excitation across kinetic barriers to realize metastable states that are thermodynamically inaccessible. Using these non-equilibrium methods, they will aim at realizing some of the most sought-after phenomena in condensed matter physics including collective charge/current ordered phases, bandwidth controlled metal to Mott insulator transitions, quantum disordered magnets such as valence bond solids and highly entangled quantum spin liquid states, and low dimensional and quantum critical electron liquids with no quasiparticle description.

Modular Quantum Systems

This success supports these ARL Core Technical Competencies:

Network and Information Sciences

Computational Sciences

The MURI topic authors and co-managers of this project are Dr. T.R. Govindan, Physics Division and Dr. T. Curcic, Air Force Office of Scientific Research.

This MURI began in FY16 and was awarded to a team led by Professor Christopher Monroe at the University of Maryland – College Park. The goal of this research is to discover and explore modularity concepts for extensibility of small high-performance multi-qubit systems to larger systems with reduction of operational complexity. A paramount challenge in exploring physical systems (qubits) suitable for quantum

information processing has been the contradictory requirement for precise manipulation of a quantum state on demand while maintaining strict isolation from the environment. Significant progress has been made in addressing this challenge. Coherence in several physical qubit types has improved by orders of magnitude. High fidelity fundamental quantum logic operations have been demonstrated. This progress has extended to multi-qubit systems involving a few (order ten) qubits. Progress continues to be made in improving coherence and fidelity. In parallel, advances have been made in connecting physically separated qubits. Key to these rapid advances has been a multi-disciplinary approach involving physics, materials science, control engineering, computer science, and mathematics, among other fields. A scientific challenge to further progress in the field has been the difficulty to add qubits and increase system size, while maintaining coherence and high-fidelity operations. System size needs to be increased before useful functionality can be explored and realized. Adding qubits increases the complexity of interactions between the qubits and makes layout, fabrication, and quantum control for high fidelity operations extremely challenging. Additional unwanted interactions introduce new qubit degrees of freedom to entangle with the environment and degrade coherence and fidelity. Modularity is a general scientific approach to address such complexity in which the system is decomposed into repeatable blocks with well-defined and controlled interfaces and interactions between the blocks and has been applied successfully to classical systems. Here, a module can be envisaged as a functional group of qubits and an interface. Exploring modularity for complex quantum systems is nascent but provides a potential extensible approach in which small numbers of high performance qubits can be extended to groups of high performance qubits and interfaces capable of precise manipulation within the group, between groups when required, and isolation from the environment and other groups.

Any quantum information processing system must balance the need for coherent control of the many interacting qubits necessary for a large-scale quantum system with decoherence rates that generally grow with system size. The objective of this research is to investigate a modular approach to constructing multi-qubit systems suitable for quantum information processing, to determine whether a modular system can achieve this balance and study the associated costs and benefits of taking the approach. In the long term, this research may overcome barriers and lead to new capabilities in the logistics, optimization, and the quantum simulation of materials.

Multi-modal Energy Flow at Atomically Engineered Interfaces

The MURI topic authors and co-managers of this project are Dr. Ralph Anthenien, Mechanical Sciences Division and Dr. Robert Mantz, Chemical Sciences Division.

This MURI began in FY16 and was awarded to a team led by Professor Donald Brenner at North Carolina State University (initially led by Professor Jon Paul Maria). The objective of this MURI is to bring chemistry, materials, surface science, electrochemistry, and physics together to characterize and understand short time-frame sub-nanoscale non-equilibrium phenomenon at and across materials interfaces, especially the flow, redistribution and partition of energy near the interface by devising and applying novel experimental, theoretical, and simulation approaches.

This success supports these ARL Core Technical Competencies:

Propulsion Sciences

Ballistics Sciences

Network and Information Sciences

The MURI team approach will be to explore, identify, and define multiple mechanisms of energy transfer/transduction at precision-engineered interfaces. Material systems that support energy transfer through lattice/molecular vibrations, plasmon-electron coupling, and chemical reactions will be studied. The synthesis, measurement, and modeling activities are co-designed to promote extreme-non-equilibrium excitations within nano-scale geometries; to observe in situ picosecond to microsecond property responses using newly developed methods; to inform new theoretical models; and to enable accurate multiscale prediction. The plan of work explores a simple, overarching, and materials-generic hypothesis: function and failure in advanced functional materials are overwhelmingly affiliated with interfaces, where the underlying mechanisms (desirable and undesirable) are regulated by or related to energy transfer/ transduction among inhomogeneous boundaries. Observing and understanding the local processes over multiple time and length scales will improve existing and design new materials systems, and to predict their performance.

Sequence-Defined Synthetic Polymers Enabled by Engineered Translation Machinery

This success supports these ARL Core Technical Competencies:

Propulsion Sciences

Protection Sciences

Materials and Manufacturing Sciences

The MURI topic authors and co-managers of this project are Dr. Dawanne Poree, Chemical Sciences Division and Dr. Stephanie McElhinny, Life Science Division.

This MURI began in FY16 and was awarded to a team led by Professor Michael Jewett at Northwestern University – Evanston. The goal of this MURI is to engineer the translation machinery to accept and polymerize non-biological monomers in a sequence-defined manner using non-traditional chain growth polycondensation chemistries (beyond amide and ester linkages).

Employing only four nucleotides and twenty amino acids, a plethora of biopolymers (e.g., proteins, DNA) with precisely-defined building block sequence gives these materials the ability to fold into higher-ordered structures capable of performing a variety of advanced functions such as information storage, self-replication, and signal transduction. The ability to extend comparable molecular-level sequence control to synthetic polymers, which have a much wider range of monomeric building blocks, has many scientific and technological implications, as it would enable precise control over structure-property relationships. Recent work has demonstrated that altering the sequence of short conjugated phenylene-vinylene oligomers can significantly modulate both electronic and optical properties. While greater complexity in function is anticipated for longer chain sequence-defined polymers, chemical routes to their synthesis have remained elusive. Conversely, biology synthesizes long sequence-defined polymers with extremely high efficiency and accuracy by employing templates to provide sequence information. More specifically, the ribosome, the workhorse of the translation machinery, is very adept at sequence-defined polymer synthesis through the successive condensation of amino acids (monomers), but primarily performs a single type of chemistry—amide bond formation via a chain-growth condensation polymerization. Co-opting the natural translation machinery to accept non-biological monomers is an attractive approach to synthesize non-biological polymers with the sequence control of biology. However, this approach is limited by cell viability constraints;

thus, in vitro engineering of the translation machinery may offer unprecedented freedom of design to modify and control ribosome chemistry.

The objective of this research is to engineer and repurpose the translation apparatus (including the ribosome and the associated factors needed for polymerization) to produce new classes of sequence-defined polymers. In the long term, this research may enable a broad range of disruptive technologies having significant impact on DoD capabilities. Sequence control at the atomic level will give the greatest possible control over the emergent, macroscopic behavior of oligomers and polymers, leading to new advanced personal protective gear, sophisticated electronics, fuel cells, advanced solar cells, and nanofabrication, which are all key to the protection and performance of soldiers.

Spin Textures and Dynamics Induced by Spin-Orbit Coupling

The MURI topic authors and co-managers of this project are Dr. Joe Qui, Electronics Division, Dr. Evan Runnerstrom (initially managed by Dr. John Prater), Materials Science Division, and Dr. Marc Ulrich, Physics Division.

This MURI began in FY16 and is led by Professor Kang Wang at University of California, Los Angles. The team consists of researchers from University of California – Irvine, California Institute of Technology, University of Nebraska, North Carolina State University, and University of Texas – Austin. The objective of this project is to strive for understanding of interfacial spin-orbit coupling (SOC) and exchange coupling in novel heterostructures and superlattices of topological insulators (TIs), 2D transition metal di-chalcogenides (TMDs), and ferro-(FM)/ferri-/antiferro (AFM)-magnetic materials. High quality heterostructures and superlattices containing TI/TMDs, TI/FM, and TI/AFM with the atomically sharp interface are to be synthesized and characterized, and these will constitute an ideal laboratory for enabling understanding of the interfacial SOC effects and relevant spin textures and dynamics.

This project will exploit the symmetry breaking and SOC-induced collective properties (i.e., magnetization, spin wave, and spin-orbit torque) in these heterostructures and superlattices to realize new types of topological matters such as magnetic Skyrmions, topological valley insulators, and topological spin wave (magnonic) crystals. It will also help facilitate the development of new emerging fields including spin-orbitronics, spin-valley-tronics, and axion electrodynamics. In addition, direct electrical field manipulation of spin or magnetization textures in these proposed systems through spin-orbit torque and magnetoelectric effects will be investigated for energy efficiency. The anticipated results of this project will broaden understandings of the fundamental science enabled by SOC, and establish suitable material frameworks for new spin-orbitronic devices in which multi-functional applications of spintronics for ultra-low power electronics at terahertz can be realized. This research will set a milestone in the spin-based applications by creating the knowledge base to enable novel, fast, and energy efficient technologies for communications and information processing.

This success supports these ARL Core Technical Competencies:

Network and Information Sciences

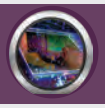
Materials and Manufacturing Sciences

Socio-Cultural Attitudinal Networks

This success supports these ARL Core Technical Competencies:

Human Sciences

Protection Sciences


Network and Information Sciences

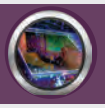
The MURI topic authors and co-managers of this project are Dr. Purush Iyer, Network Sciences Division and Dr. Lisa Troyer, Life Sciences Division.

This MURI began in FY16 and was awarded to a team led by Professor Larry Davis at the University of Maryland (initially led by Professor V. S. Subrahmanian). The goal of this MURI is two fold: (1) develop social science theories to understand latent communication among a small group of adversaries engaged in an effort to deceive, and (2) develop multi-media analytics tools that formalize those social science theories as algorithms which can aid an observer who is not steeped in the local culture. While driven by practical problems, the objectives of the proposed work is not only to drive the development of new social science theories, but also to drive algorithmic advances in reasoning about joint probability distributions that arise from modeling uncertainties in human actions, speech, gestures, and intentions.

Active MURI's that began in FY15

Advanced 2D Organic Networks

This success supports these ARL Core Technical Competencies:


Network and Information Sciences

Materials and Manufacturing Sciences

The MURI topic authors and co-managers of this project are Dr. Chakrapani Varanasi, Materials Sciences Division and Dr. Dawanne Poree, Chemical Sciences Division.

This MURI began in FY15 and was granted to a team led by Professor William Dichtel at Cornell University. The objective of this research is to create stable, free-standing, single-monomer-thick 2D crystalline organic polymer nanosheets/covalent organic frameworks (COFs) with designed electronic (conductivity, mobility, charge storage), optical (resonances, nonlinearities), and structural properties.

The team will combine mechanistic studies, theory, microscopy, and spectroscopy to gain fundamental insight into the 2D polymerization processes. Specifically the team will address the challenges in 2D COF synthesis and characterization by focusing on the following three major research thrusts: (1) exploration of nucleation, bond exchange, and polymerization of 2D COFs to improve their long-range order and morphological form and isolate 2D COFs as single crystals; (2) investigation of new conjugated linkage chemistries, topologies, and doping strategies to impart extensive electronic delocalization and useful optical and electronic properties; and (3) fabrication of new hybrid device heterostructures based on the interfacing of 2D COFs with newly emerging 2D inorganic materials such as transition metal dichalcogenides.

Emulating the Principles of Impulsive Biological Force Generation

The MURI topic authors and co-managers of this project are Dr. Samuel Stanton, Mechanical Sciences Division and Dr. Robert Kokoska, Life Sciences Division.

This MURI began in FY15 and was awarded to a team led by Professor Sheila Patek of Duke University. The objective of this MURI is to establish a unified theory

for understanding biological and engineered impulsive systems. The MURI team will approach the objective using a thermodynamic framework linked to impulsive performance. This will require integrating mathematical analysis, tests of biological impulsive systems, and synthesis of impulsive materials and mechanisms. The thermodynamic framework consists of five phases: (1) chemical energy conversion in cellular biological systems that potentially circumvent the force-velocity tradeoffs of actin-myosin muscle mechanisms; (2) actuation tuned to spring loading through novel engineering implementations and informed by analyses of muscular and cellular thermodynamics; (3) potential energy storage through a diversity of biological materials, scales and geometries to inform synthetic elastic design; (4) rapid conversion from potential to kinetic energy (power amplification) – a defining feature of impulsive systems – through analyses of rate-dependence in biological materials/geometries, the mechanics of biological linkages and latches, and their directed synthesis into novel impulsive designs; and, (5) environment-system interactions through rigorous tests of the effects of environmental substrates and geometries, internal dissipation and reset mechanisms for repeated use and mitigation of failure due to environmental forces. This research effort will lay the foundations for scalable methods for generating forces for future actuation and energy storing structures and materials.

This success supports these ARL Core Technical Competencies:

Propulsion Sciences

Ballistics Sciences

Materials and Manufacturing Sciences

Engineering Exotic States of Light with Superconducting Circuits

The MURI topic authors and co-managers of this project are Dr. T.R. Govindan, Physics Division and Dr. Joe Qui, Electronics Division.

This MURI began in FY15 and was awarded to a team led by Professor Andrew Houck at Princeton University. The goal of this MURI is to initiate significant new experimental and theoretical explorations to harness recent breakthroughs in superconducting systems and to demonstrate useful new states of light that can be brought to bear on broader goals in sensing, measurement, simulation, and computation. If successful, this research may lead to new tools for metrology, could provide key insight into non-equilibrium quantum systems, and will provide new resources for quantum communication and sensing.

Quantum optics, particularly in the domain of cavity quantum electrodynamics, provides a pathway to create and use large macroscopic quantum states with photons. Such states have been difficult to generate because atoms trapped in a cavity provide only weak nonlinearity to mediate photon-photon interactions, high photon loss introduces decoherence, low photon collection and detection efficiency decrease success probability, among other challenges. On the other hand, recent progress in superconducting qubits and high-quality microwave cavities for quantum computing has enabled orders of magnitude improvements in coherence, fast single shot high-fidelity readout, high-fidelity quantum operations, low photon loss, and better understanding of decoherence mechanisms. These advances have enabled early experiments that have demonstrated the creation of high-fidelity coherent states with several tens of photons. In addition, the new generation of superconducting devices opens up the opportunity for the exploration of new regimes of quantum optics involving quantum states of 100s of

This success supports these ARL Core Technical Competencies:

Network and Information Sciences

Computational Sciences

photons. Further advances are possible if, in addition to the physics of quantum optics, advanced microwave circuit engineering is brought to bear on the regime of low-power microwave signals to improve coherence and function, and materials science is employed to determine relationships between decoherence and defects in materials, surface chemistry, and interface quality. In turn, the superconducting systems and the quantum states created in them could also be used as sensitive probes of materials behavior, in particular of the origin and sources of decoherence and dissipation mechanisms.

The multidisciplinary research team led by Professor Houck combines the efforts of physicists and engineers who will develop the theoretical and experimental tools to establish new regimes of quantum optics using superconducting circuits. The new states of light established in this program provide new tools for metrology, could provide key insight into non-equilibrium quantum systems, and in the long term may lead to applications in quantum communication and sensing.

Fractional PDEs for Conservation Laws and Beyond: Theory, Numerics, and Applications

This success supports these ARL Core Technical Competencies:

Computational Sciences

The MURI topic author and manager of this project is Dr. Joe Myers, Mathematical Sciences Division.

This MURI began in FY15 and is awarded to a team led by Professor George Karniadakis at Brown University. The goal of this research is to develop a new rigorous theoretical and computational framework enabling end-to-end fractional modeling of physical problems governed by conservation laws in large-scale simulations.

Despite significant progress over the last 50 years in simulating complex multiphysics problems using classical (integer order) partial differential equations (PDEs), many physical problems remain that cannot be adequately modeled using this approach. Examples include anomalous transport, non-Markovian behavior, and long-range interactions. Even well-known phenomena such as self-similarity, singular behavior, and decorrelation effects are not easily represented within the confines of standard calculus. This project seeks to break this deadlock by developing a new class of mathematical and computational tools based on fractional calculus, advancing the field in specific areas of computational mechanics. The fractional order may be a function of space-time or even a distribution, opening up great opportunities for modeling and simulation of multiscale and multiphysics phenomena based on a unified representation. Hence, data-driven fractional differential operators will be constructed that fit data from a particular experiment, including the effect of uncertainties, in which the fractional PDEs (FPDEs) are determined directly from the data.

The work is addressing the fundamental issues associated with the construction of fractional operators for conservation laws and related applications. An integrated framework is being pursued that proceeds from the initial data-driven problem to ultimate engineering applications. This general methodology will allow the development of new fractional physical models, testing of existing models, and assessment of numerical methods in terms of accuracy and efficiency. The integrated framework is based on a dynamic integration of five areas: (1) mathematical analysis of FPDEs; (2)

numerical approximation of FPDEs; (3) development of fast solvers; (4) fractional order estimation and validation, from data; and (5), prototype application problems.

Imaging and Control of Biological Transduction using Nitrogen Vacancy Diamond

The MURI topic authors and co-managers of this project are Dr. Frederick Gregory, Life Sciences Division and Dr. Paul Baker, Physics Division.

This MURI began in FY15 and was awarded to a team led by Professor Ronald Walsworth at Harvard University. The goal of this MURI is to further develop nitrogen vacancy nanodiamonds as non-biological quantum sensors and engineer a biological interface for actuating biological processes.

The nitrogen vacancy center lattice defect in diamond nanoparticles (NV-diamond) can retain activity in biological environments. Current applications of NV-diamond include quantum computing, nanoscale magnetometry, super-resolution imaging and atomic scale magnetic resonance imaging. These state of the art applications involve NV-diamonds implanted in substrates; however recent breakthroughs have allowed isolated nano-diamond particles to be used as biosensing intracellular quantum probes for thermometry and bacterial tracking as well as extracellular quantum probes of ion channel operation. A key reason for NV-diamond sensitivity, including in the emerging biosensing applications, is that the spectral shape and intensity of optical signals from NV-diamond are sensitive to external perturbation by strain, temperature, electric fields and magnetic fields. Biological sensory transduction relies upon highly evolved ion channel-based mechanisms that involve transducing environmental energy into a bioelectrical signal for intercellular communication. The recent demonstrations of NV-diamond's extreme sensitivity and localization now provide new research opportunities for transitioning NV-diamonds from passive sensors to novel biophysical interfaces whose perturbed energy emission can be used as a signal to control or modify sensory transducer molecular physiology and intra- and inter-cellular signaling.

This multidisciplinary project four closely-coupled aims: (1) to optimize nitrogen vacancy nanodiamond synthesis, (2) to realize stable, biocompatible nanodiamond surface functionalizations, (3) to advance nitrogen vacancy sensitivity to chemical and biological systems and (4) to enable nitrogen vacancy-based manipulation of biological transduction. Systematically studying the integration of nitrogen vacancy nanodiamonds with reconstituted or native ion channels will lead to greater understanding and more importantly, create a new paradigm for exogenous control of biological transduction events and the ability to uncover fundamental mechanisms with unprecedented spatial and temporal resolution. This endeavor may lead to significant scientific breakthroughs in understanding how to develop and control quantum systems capable of interfacing with, and controlling, biological systems. If successful, this research may improve future Army capabilities ranging from advanced artificial intelligence systems, early diagnosis and effective treatment of neurological disorders at the cellular level, novel human-machine interfaces, and antidotes to neurotoxins and pathogens.

This success supports these ARL Core Technical Competencies:

Protection Sciences

Network and Information Sciences

Materials and Manufacturing Sciences

Multi-Scale Responses in Organized Assemblies

This success supports these ARL Core Technical Competencies:

Protection Sciences

Materials and Manufacturing Sciences

The MURI topic authors and co-managers of this project are Dr. Dawanne Poree, Chemical Sciences Division and Dr. Evan Runnerstrom (initially managed by Dr. John Prater), Materials Science Division.

This MURI began in FY15 and was awarded to a team led by Professor Sankaran Thayumanavan, at University of Massachusetts - Amherst. The goal of this MURI is to understand how a molecular level detection can be propagated across a macroscopic material to affect a global property change that spans multiple length and time scales, and connecting these multi-scale events to realize signal amplification.

Living systems are complex systems capable of receiving and using information, interacting with each other and their environment, and performing specific functions in response to stimuli occurring at multiple length and time scales. These sophisticated, innate behaviors are essential for survival, and can be extremely valuable in non-natural systems. A variety of synthetic systems have been engineered to respond to specific stimuli; however, the dynamics of the chemical and material processes and interactions occurring at multiple length and time scales throughout the signal-propagate-response pathway are inadequately understood to rationally design autonomous, “living” systems. The daunting challenge toward synthetic “living” systems is predictably propagating a molecular level change, generated through the selective sensing of a trigger, into a readily discernible macroscopic change in a material’s fundamental properties. This can only be addressed by developing a fundamental understanding of the chemical processes that occur at multi-scale levels – from molecular to nano to macroscopic length scales and from nanoseconds to hours. The inherent complexity involved in connecting these length scales, and the propagation and amplification of the resulting signals, requires a cohesive, multidisciplinary approach.

The integrated research plan led by Professor Thayumanavan is comprehensive and addresses each of the key elements needed to understand the fundamental multi-scale responses of adaptive systems occurring across length and time scales. The research is exploiting a variety of material platforms/approaches, including liquid crystal orientation, responsive amphiphiles, depolymerization, and biological/abiological composites with non-equilibrium molecular release to address propagation and amplification at multiple length scales. Each system approach is innovative, well-formulated, and focused on a complete understanding of the basic research principles controlling each approach. A variety of triggers will be considered throughout the effort including pH, temperature, redox, light, and enzymes. A key part of this effort is the ability to monitor dynamic changes during the cooperative reorganization processes at the interface, and this is addressed by integration of novel characterization techniques such as in situ liquid cell transmission electron microscopy. If successful, this fundamental research may ultimately enable Army-relevant technologies in stimuli-responsive systems such as self-decontaminating materials, controlled release for hazardous materials management or drug delivery, and responsive systems for self-healing and smart materials.

Network Science of Teams

The MURI topic author and manager of this project is Dr. Edward Palazzolo, Network Sciences Division.

This MURI began in FY15 and was awarded to Professor Ambuj Singh of the University of California at Santa Barbara, with participation from researchers at University of Southern California, University of Illinois at Urbana-Champaign, Northwestern University, and MIT. These seven faculty provide an excellent balance of multidisciplinary scholars from sociology, cognitive and social psychology, health and behavioral sciences, computer science, statistics, controls and dynamical systems, and network science. This MURI will advance the development of the Network Science of Teams by creating quantitative, network-based models of adaptive team behavior. This research will produce methods to optimize team performance under different contexts and resource constraints. The three thrusts of this research effort include (1) teams as networks of interacting entities, (2) analysis and models of dynamic team behavior over task sequences, and (3) the network science of teams-of-teams or multi-team systems. The overarching objectives of this research are to build quantifiable informative models of team behavior as dynamical systems interacting over multiple networks, to develop rigorous models that relate interaction patterns and network evolution to task performance, to break new ground in the learning of optimal design of teams for complex tasks, and to advance social science theories of team performance. This MURI will have a significant impact for the Army and DoD with respect to how it conducts its work in teams in that results from this research may help the Army and joint forces assemble more effective teams and teams of teams, and provide guidance on task sequencing to support their highest goals.

This success supports these ARL Core Technical Competencies:

Human Sciences

Protection Sciences

Network and Information Sciences

Noncommutativity in Interdependent Multimodal Data Analysis

The MURI topic authors and co-managers of this project are Dr. Cliff Wang (initially managed by Dr. Liyi Dai), Computing Sciences Division and Dr. T.R. Govindan, Physics Division.

This MURI began in FY15 and was awarded to a team led by Professor Rayadurgam Srikant at the University of Illinois at Urbana-Champaign (initially led by Professor Negar Kiyavash). The goal of this research is to establish a new comprehensive information theory for data analysis in noncommutative information structures intrinsic to hierarchical representations, distributed sensing, and adaptive online processing. Methods will be developed based on a novel theory in conjunction with the latest theories of information, random matrices, free probability, optimal transport, and statistical machine learning. They will be applied to the technical domains of causal inference, adaptive learning, computer vision, and heterogeneous sensor networks, and will be validated on real-data test beds including: (1) human action and collective behavior recognition, and (2) crowd-sourcing in a network of brain-machine interfaces. The framework will provide answers to questions such as: What are the fundamental performance limits for noncommutative information collection and processing

This success supports these ARL Core Technical Competencies:

Network and Information Sciences

Computational Sciences

systems? What is the effect of side information on noncommutative information structures? How can low complexity proxies for performance be defined that approximate or bound noncommutative performance limits? How can noncommutativity of adaptive measurements be exploited to improve fusion, processing, and planning for distributed sensing systems? When do sequential or partially ordered designs offer significant performance gains relative to randomized designs like compressive sensing?

The approaches for extracting knowledge from complex irreversible partially ordered information structures include but are not limited to introduction of information divergence measures over noncommutative algebras, noncommutative relative entropy measures, and estimation techniques for such measures for high-dimensional data. Accounting for noncommutative structures will result in fundamentally new ways of fusing ordered, directed, or hierarchical organized information to support timely decisions at the appropriate level of granularity. Humans learn actively and adaptively, and their judgments about the likelihood of events and dependencies among variables are strongly influenced by the perception of cause and effect, whereas man-made systems only employ correlation-type symmetric measures of dependencies. Research will lead to the development of a theory of decentralized information sharing, causal inference, and active learning inspired by human decision making. Establishment of such a theory for sensing and data processing and application of it to grand challenges in computer vision and brain-computer interfaces will provide new capabilities, including improved time-sensitive, dynamic, multi-source information processing, actuation, and performance prediction guarantees.

Active MURIs that began in FY14

Attosecond Electron Dynamics

This success supports these ARL Core Technical Competencies:

Propulsion Sciences

Ballistics Sciences

Protection Sciences

The MURI topic authors and co-managers of this project are Dr. James Parker, Chemical Sciences Division and Dr. Marc Ulrich (initially managed by Dr. Richard Hammond), Chemical Sciences Division.

This MURI began in FY14 and was awarded to a team led by Professor Stephen Leone at the University of California - Berkeley. The goal of this MURI is to use attosecond light pulses to study the electron dynamics of atoms and small molecules.

Attosecond dynamics is a new field of scientific investigation which allows one to examine dynamics phenomena on the natural timescale of electronic processes in atoms, molecules, and materials. The timescale of microscopic dynamics in quantum systems occur at a timescale about one order of magnitude less than those for less-energetic processes, such as valence electronic transitions in molecules and semi-conductor materials. A recent scientific breakthrough known as double optical gating has led to the production of broadband laser pulse widths as short as 67 attoseconds, making direct observation of a variety of electronic phenomena possible in real time. Thus, now there exist opportunities to examine a variety of electron-dynamics phenomena that arise from electronic motions in molecules on the attosecond timescale.

The objective of this research is to harness attosecond pulses of electromagnetic energy to probe matter (e.g., atoms, molecules, plasmas) at attosecond time scales for the real-time observation, control, and understanding of electronic motion in atoms,

molecules, and materials. If successful, this research may lead to new synthesis methods, such as plasmonically-enhanced catalysis for the direct reduction of CO2 to create fuels, new schemes and manufacturing methods for solar photovoltaics, nano-catalysts for fuel combustion, and high-density specific impulse propellants.

Force-activated Synthetic Biology

The MURI topic authors and co-managers of this project are Dr. Stephanie McElhinny, Life Sciences Division and Dr. David Stepp, Materials Science Division.

This MURI began in FY14 and was awarded to a team led by Professor Margaret Gardel at the University of Chicago. The goal of this MURI is to understand the mechanisms by which biochemical activity is regulated with mechanical force and reproduce the mechanisms in virtual and synthetic materials.

A critical aspect of synthetic biology systems is the targeted and controlled activation of molecules affecting biological function. Molecules can be activated by a variety of different signals, including chemical, optical and electrical stimuli, and synthetic biological circuits responsive to each of these stimuli have been successfully assembled. In recent years, the ability of mechanical force to serve as a biological signal has emerged as a unique and unexpected facet to biological activation. The rapidly growing field of mechanotransduction is beginning to reveal an extraordinary diversity of mechanisms by which mechanical forces are converted into biological activity. This field has been heavily influenced and driven through ARO funded research, including a prior MURI[4-7]. Despite these rapid advances, mechanophores have never been incorporated into advanced synthetic material. This research area provides an exceptional opportunity to integrate biological activation by mechanical force into the growing toolbox of synthetic biology, and to establish unprecedented paradigms for the incorporation of highly specific force activation and response into new materials.

The objective of this research is to elucidate the molecular mechanisms by which living cells regulate intracellular biochemical activity with mechanical force, to reproduce and analyze these force-activated phenomena in synthetic and virtual materials, and to design and exploit optimized synthetic pathways with force-activated control. If successful, this research may dramatically influence future advances in engineered biological systems, materials synthesis and fabrication, and force-responsive and adaptive bio-mimetic material systems.

This success supports these ARL Core Technical Competencies:

Protection Sciences

Materials and Manufacturing Sciences

[4]*Potisek SL, Davis DA, Sottos NR, White SR, Moore JS. (2007). Mechanophore-linked addition polymers. J Am Chem Soc.129:13808-9.*

[5]*Davis DA, Hamilton A, Yang J, Cremar LD, Van Gough D, Potisek SL, Ong MT, Braun PV, Martínez TJ, White SR, Moore JS, Sottos NR. (2009). Force-induced activation of covalent bonds in mechanoresponsive polymeric materials. Nature. 459:68-72.*

[6]*Lenhardt JM, Ong MT, Choe R, Evenhuis CR, Martinez TJ, Craig SL. (2010). Trapping a diradical transition state by mechanochemical polymer extension. Science. 329:1057-60.*

[7]*Burnworth M, Tang L, Kumpfer JR, Duncan AJ, Beyer FL, Fiore GL, Rowan SJ, Weder C. (2011). Optically healable supramolecular polymers. Nature. 472:334-7.*

Innovation in Prokaryotic Evolution

The MURI topic authors and co-managers of this project are Dr. Micheline Strand, Life Sciences Division and Dr. Joe Myers (initially managed by Dr. John Lavery), Mathematical Sciences Division.

This MURI began in FY14 and was awarded to a team led by Professor Michael Lynch at Indiana University - Bloomington. The goal of this MURI is to model evolution in nutrient-deprived bacterial cultures, and then characterize changes in the genetic, metabolic, and social networks to create models that reflect the complexities of group evolution.

This success supports these ARL Core Technical Competencies:

Human Sciences

Protection Sciences

Computational Sciences

Classical Darwinian evolution selects for individuals that are better than others of their species in critical areas associated with reproductive fitness. For example, giraffes are selected for longer necks and cheetahs are selected for running speed. Similarly, single-celled organisms growing in rich media are selected for their ability to reproduce more quickly. In contrast, organisms that have run out of food can no longer simply improve at what they are already able to do; they are forced to innovate new methods to exploit previously untapped resources. In times of scarcity, even unicellular organisms rapidly evolve into complex societies with assorted subpopulations formed with unique and specialized skills. It is no longer an effective strategy to grow faster during starvation. In short, evolution during lean times requires the group to evolve as a whole, as each individual competes, cooperates, and depends on other members of the group.

The objective of this research is to develop a model of evolution in isolated independent cultures of organisms that are starving for months or years, and then model change in the genetic, epigenetic, transcriptomic, proteomic, metabolomic, and social networks to create experimentally-validated, mathematically-rigorous, and predictive models that accurately reflect the real complexities of group evolution. In the long term, the results of this research may lead to new applications for safer, economical food and water storage, new mechanisms to control and kill pathogens that will impact wound healing, diabetes, heart disease, dental disease, and gastrointestinal disease.

Multiscale Mathematical Modeling and Design Realization of Novel 2D Functional Materials

This success supports these ARL Core Technical Competencies:

Propulsion Sciences

Materials and Manufacturing Sciences

Computational Sciences

The MURI topic authors and co-managers of this project are Dr. Joe Myers, Mathematical Sciences Division and Dr. Chakrapani Varanasi, Materials Science Division.

This MURI began in FY14 and was awarded to a team led by Professor Mitchell Luskin of the University of Minnesota. This research is co-managed by the Mathematics and Materials Science Divisions. The objective of this project is to develop efficient and reliable multiscale methods to couple atomistic scales to the mesoscopic and the macroscopic continuum for layered heterostructures. Layered heterostructures represent a dynamic new field of research that has emerged from recent advances in producing single atomic layers of semi-metals (graphene), insulators (boron nitride) and semiconductors (transition metal dichalcogenides). Combining the properties of these layers opens almost unlimited possibilities for novel devices with desirable, tailor-made electronic, optical, magnetic, thermal and mechanical properties. The vast range of possible choices requires theoretical and computational guidance of experimental searches; experimental discovery can in turn inform, refine and constrain the theoretical predictions.

The proposed research will develop efficient and reliable strongly-linked multiscale methods for coupling several scales based on a rigorous mathematical basis. Specifically: 1) The rigorous coupling of quantum to molecular mechanics will be achieved by properly taking into account the mathematics of aperiodic layered structures. 2) The coupling of atomistic-to-continuum will be achieved by methods

that can reach the length scales necessary to include long-range elastic effects while accurately resolving defect cores. 3) New accelerated hybrid molecular simulation methods, specially tailored for the weakly interacting van der Waals heterostructures, will be developed that can reach the time scales necessary for synthesis and processing by CVD and MBE. 4) The simulations will be linked to macro and electromagnetic modelling to understand the physics and bridge to experimental investigation.

The challenge of modeling layered heterostructures will promote the development of strongly-linked multiscale models capable of handling many other materials systems with varied applications, including composites, meta-atoms (atomically engineered structures), and bio-materials that are of interest to the Army.

Multistep Catalysis

The MURI topic authors and co-managers of this project are Dr. Robert Mantz, Chemical Sciences Division and Dr. David Stepp, Materials Science Division.

This MURI began in FY14 and was awarded to a team led by Professor Shelley Minteer at the University of Utah. The goal of this MURI is to enable multi-step chemical reactions through the rational design of architectures that control the spatial and temporal pathways of precursors, intermediates, and products.

The Krebs cycle is an exquisite example of a regulated enzyme cascade which biological systems use to precisely control charge and reactant transport to produce energy for the cell. Conversely, man-made systems typically involve a series of conversions with intermediate purification steps to achieve a desired product, with yield losses that compound with each step. The current approach to achieve multi-step reactions in a single reactor is an arbitrary combination of multiple catalysts that is likely to lead to poor yield with unreacted intermediates or byproducts of reactants that have reacted with the incorrect catalysts. Recent breakthroughs in materials synthesis, such as self-assembly and lock-and-key type architectures, offer control of surface arrangement and topology that enable a much more effective approach to achieving multi-step reactions through control of spatial and temporal transport of reactants, electrons, intermediates, and products.

The objective of this research is to establish methodologies for modeling, designing, characterizing, and synthesizing new materials and structures for the design and implementation of multi-step catalysis. In particular, integrated catalytic cascades will be created from different catalytic modalities such that novel scaffolding and architectures are employed to optimize selectivity, electron transfer, diffusion, and overall pathway flux. If successful, this research will provide unique paradigms for exploiting and controlling multistep catalysis with dramatically enhanced efficiency and complexity. In the long term, the results may lead to new energy production and storage technologies.

This success supports these ARL Core Technical Competencies:

Propulsion Sciences

Protection Sciences

Materials and Manufacturing Sciences

New Theoretical and Experimental Methods for Predicting Fundamental Mechanisms of Complex Chemical Processes

This success supports these ARL Core Technical Competencies:

Propulsion Sciences

Protection Sciences

Materials and Manufacturing Sciences

The MURI topic authors and co-managers of this project are Drs. Ralph Anthenien and Samuel Stanton, Mechanical Sciences Division.

This MURI began in FY14 and was awarded to a team led by Professor Donald Thompson of the University of Missouri – Columbia. The objective of this MURI is to develop new approaches to predictive models for complex, reacting systems. It will develop supporting fundamental theory, perform supporting experiments, and validate resultant models and methods. The goal is to develop computationally efficient, predictive, accurate, robust methods to predict the molecular energy hypersurface, as well as relevant pathways and bifurcation topology for reacting coordinates.

The effort will accomplish the objectives via a comprehensive research program that will design efficient methods to predict and control the behavior of complex chemical reactions, such as combustion. Complexity is the salient challenge facing modern physical chemistry, and the proposed research will yield fundamental new methods to directly address the complexity of chemical reactions - from ab initio principles to the collective evolution of chemical populations. The research program is based on two ideas: (1) It is not necessary to describe or even know all the details, only those directly involved in the relevant pathway(s) from reactants to products, and (2) it is essential to understand the role of fluctuations in the reaction rate, such as those that can be induced by the energetic environment and the many intermediates in combustion processes. The robust and accurate methods developed will determine the critical, emergent behaviors of complex overall reactions in non-equilibrium environments. They will accurately describe how a set of reactants undergoes sequential, branching reactions, passing through many transition states and transient species, to reach a final set of stable products. To gain an understanding of the role of fluctuations in reaction rates far from equilibrium, the researchers will focus on extracting information from the detailed dynamics of molecular species that are responsible for the fluctuations and, ultimately, the limits of traditional chemical kinetics. A synergistic approach will be undertaken for these overarching challenges that integrates the full range of rigorous fundamental theoretical methods. The specific objectives of the project leverage the complexity of kinetic phenomena, which are typically nonlinear, stochastic, multi-dimensional, strongly coupled, and can persist far from equilibrium by extreme variations in intensive properties. Some of the sub-objectives will be to: (1) fully leverage the predictive capabilities of state-of-the-art electronic structure theory. (2) Gain a better understanding of how complex chemistry occurs at a microscopic level over wide ranges of temperature and pressure. (3) Identify and control relevant dynamical variables that can be probed experimentally. (4) Elucidate the role of statistical fluctuations in energy and matter on chemistry by analyzing the underlying nonlinear dynamics and reaction networks. (5) Design tractable theoretical and computational methods with immediate experimental links and reduced dimensionality without diminishing predictive capabilities. (6) Formulate connections among complexity theories, nonlinear dynamics, network theory, and chemistry. (7) Seek kinetic control of chemical and energetic phenomena on a macroscopic (rather than microscopic) level using nonlinear dynamics, optimal control, large deviations, and network theory.

Ultracold Molecular Ion Reactions

The MURI topic authors and co-managers of this project are Dr. Paul Baker, Physics Division and Dr. James Parker, Chemical Sciences Division.

This MURI began in FY14 and was awarded to a team led by Professor Eric Hudson at the University of California - Los Angeles. The goal of this MURI is to design, create, and exploit molecular ion traps to explore precision chemical dynamics and enable the quantum control of ultracold chemical reactions.

Investments quantum computing and precision metrology have led to the development of molecular ion trap technology. These advances provide scientific opportunities that could be exploited to enable new methods for the study and control of chemical reactions. Recent scientific breakthroughs have been achieved in ultra-cold chemistry with neutrals, suggesting that ion chemistry would provide similar opportunities for an emerging new field. In addition, work in quantum information has led to the development of new types of arrayed micro-fabricated ion traps. Ion trap technology adds novel capabilities to molecular ion research, enabling new research opportunities in materials science, condensed-matter physics, chemistry, and biochemistry. In particular, ion traps offer dramatic improvements in chemical sensing at the single-ion level. Compared with molecular neutrals, trapped molecular ions offer interaction times much longer than what is possible in beam experiments; state preparation and readout is potentially cleaner; and Coulomb interactions with co-trapped atomic ions allow for general species-independent techniques.

The objective of this research is to develop and create molecular ion traps to exploit long interrogation time to study molecular ion chemistry, utilize extended interaction times and dipolar interactions in novel quantum control scenarios, improve chemical sensing using single-ion detection, and integrate the traps with various detectors. This research could ultimately leave to dramatically improved methods for creating and studying quantum dots, energetic compounds, biological reactions, and tools for detection of trace molecules.

This success supports these ARL Core Technical Competencies:

Propulsion Sciences

Protection Sciences

Materials and Manufacturing Sciences

Understanding the Skin Microbiome

The MURI topic authors and co-managers of this project are Dr. Virginia Pasour, Mathematical Sciences Division and Dr. Robert Kokoska (initially managed by Dr. Wallace Buchholz), Life Sciences Division.

This MURI began in FY14 and was awarded to a team led by Professor David Karig of the Applied Physics Lab at the Johns Hopkins University. The goal of this research is to develop a fundamental understanding of the forces shaping skin microbial communities across a range of spatial scales and to show how this understanding can be used to identify disease risk, predict disease outcomes and develop tools for disease prevention.

Human skin harbors diverse bacterial communities that vary considerably in structure between individuals and within individuals over time. The extent of this variability and its implications are not fully understood, nor is it known whether it is possible to predict what types of bacteria one is likely to find on the skin of a given individual. As a result,

This success supports these ARL Core Technical Competencies:

Human Sciences

Protection Sciences

Computational Sciences

there are no effective tools to predict individuals more likely to acquire skin bacterial infections, then determine the efficacy of forensic analyses based on skin bacterial communities, nor to design novel strategies to limit the effective colonization of skin by pathogens. This project brings a variety of disciplines to bear on the problem: spatially explicit sampling, metagenomics, and bioinformatics will be used to characterize skin microbial communities at intermediate and large spatial scales. Molecular biology, analytical chemistry and synthetic biology will be used to probe smaller-scale processes that ultimately lead to larger-scale patterns. Ecological modeling will be used to integrate small-scale processes with large-scale patterns in order to arrive at a quantitative and predictive framework for interpreting the human skin microbiome. A series of models concentrating on four grand challenges will be built, tested and refined: (1) predicting microbiome composition based on environmental conditions, host state and microbe exposure patterns, (2) identifying microbiome composition through volatile sensing, (3) identifying disease risk through analysis of current state and anticipation of state changes, e.g., due to upcoming activities or events, and (4) novel approaches for mitigating skin disease (e.g., optimal design of avoidance behavior, robustly engineered skin microbiomes). The results of this work will enable the manipulation of the skin microbiome in order to facilitate identification of allies, discourage bites of flying insects, predict skin disease, and as-yet-unimagined applications.

Active MURIs that began in FY13

Adversarial and Uncertain Reasoning for Adaptive Cyber Defense: Building the Scientific Foundation

This success supports these ARL Core Technical Competencies:

Protection Sciences

Network and Information Sciences

Computational Sciences

The MURI topic author and manager of this project is Dr. Cliff Wang, Computing Sciences Division.

This MURI began in FY13 and was awarded to a team led by Professor Sushil Jajodia of George Mason University. Adaptive defense mechanisms are essential to protect our nation's critical infrastructure (computing, communication, and control) from sophisticated adversaries who may stealthily observe defense systems and dynamically adapt their attack strategies. This research aims to create a unified scientific foundation to enable the design of adaptive defense mechanisms that will maximize the protection of cyber infrastructure while minimizing the capabilities of adversaries.

The research will leverage recent advances in security modeling, network science, game theory, control theory, software system and network protocol security to create the scientific foundation, which may include general models for defense mechanisms and the systems they protect as well as irrational and rational adversaries. This research will develop a new class of technologies called Adaptive Cyber Defense (ACD) that will force adversaries to continually reassess, reengineer and relaunch their cyber attacks. ACD presents adversaries with optimized dynamically-changing attack surfaces and system configurations, thereby significantly increasing the attacker's workloads and decreasing their probabilities of success.

Artificial Cells for Novel Synthetic Biology Chassis

The MURI topic authors and co-managers of this project are Dr. Stephanie McElhinny, Life Sciences Division and Dr. Dawanne Poree (initially managed by Dr. Jennifer Becker), Chemical Sciences Division.

This MURI began in FY13 and was awarded to a team led by Professor Neal Devaraj at the University of California - San Diego. The goal of this MURI is to understand how biological and biomimetic synthetic cellular elements can be integrated to create novel artificial cells with unprecedented spatial and temporal control of genetic circuits and biological pathways.

The field of synthetic biology aims to achieve design-based engineering of biological systems. Toward this goal, researchers in the field are identifying and characterizing standardized biological parts for use in specific biological organisms. These organisms serve as chassis for the engineered biological systems and devices. While single-celled organisms are typically used as synthetic biology chassis, the complexity of even these relatively simple organisms presents significant challenges for achieving robust and predictable engineered systems. A potential solution is the development of minimal cells which contain only those genes and biomolecular machinery necessary for basic life. Concurrent with recent advances toward minimal biological cells, advances have also been made in biomimetic chemical and material systems, including synthetic enzymes, artificial cytoplasm, and composite microparticles with stable internal compartments. These advances provide the scientific opportunity to explore the integration of biological and biomimetic elements to generate an artificial hybrid cell that for the first time combines the specificity and complexity of biology with the stability and control of synthetic chemistry.

The objective of this MURI is to integrate artificial bioorthogonal membranes with biological elements to create hybrid artificial cells capable of mimicking the form and function of natural cells but with improved control, stability, and simplicity. If successful, these artificial cells will provide a robust and predictable chassis for engineered biological systems, addressing a current challenge in the field of synthetic biology that may ultimately enable sense-and-respond systems, drug-delivery platforms, and the cost-effective production of high-value molecules that are toxic to living cells (e.g., alternative fuels, antimicrobial agents).

This success supports these ARL Core Technical Competencies:

Protection Sciences

Materials and Manufacturing Sciences

Control of Complex Networks

The MURI topic authors and co-managers of this project are Dr. Randy Zachery, Network Sciences Division and Dr. Samuel Stanton, Mechanical Sciences Division.

This MURI began in FY13 and was awarded to a team led by Professor Raissa D'Souza of the University of California – Davis. The goal of this MURI project is to develop rigorous principles to predict and control behaviors of systems made of interdependent networks. This will be accomplished through an interdisciplinary approach synthesizing mathematical theories from statistical physics, control theory, nonlinear dynamics, game theory, information theory, system reliability theory, and operations research. The results will be informed and validated by empirical studies of real-world systems from

This success supports these ARL Core Technical Competencies:

Network and Information Sciences

nanoscale mechanical oscillators, to collections of interdependent critical infrastructure systems, to data on coalitions and conflict in primate societies, to longitudinal data on the evolution of political networks of nation states and task-oriented social networks in open source software. The focus is to develop new approaches that exploit network interdependence for network control, and this diversity of empirical testbeds is central to developing robust theoretical principles and widely applicable methods.

It is expected that this MURI will lead to (1) network interventions that prevent cascades of failure in critical infrastructures, (2) novel control schemes relying on control actions and local interventions, (3) rigorous principles for multi-modal recovery of heterogeneous systems, (4) shaping human social response via designed incentives that align human behavior with the capabilities of technological networks, (5) design of networks of nonlinear nanoelectromechanical oscillators that exploit coupling and nonlinearity to create coherent motion, (6) new mathematical structures for representing and analyzing networks-of-networks, especially with respect to control theory, and (7) fundamental bounds on controllability of interdependent networks and rigorous techniques to identify which network layers are easiest to steer.

The anticipated impact on DoD Capabilities is broadly applicable to controlling a disparate collection of autonomous agents interacting through numerous networks in noisy, dynamic environments with a myriad of time-scales and length-scales. Results can be applied to security (and restoration) of critical infrastructures, supply chains, political alliance dynamics (including upheavals such as Arab Spring), conflict, risk, social dynamics, and collective action. It is also reasonable to expect that there will be new levels of nanoscale functionality in the NEMs device developed, enabling new technologies and devices.

Materials with Extraordinary Spin/Heat Coupling

This success supports these ARL Core Technical Competencies:

Propulsion Sciences

Materials and Manufacturing Sciences

The MURI topic authors and co-managers of this project are Dr. Chakrapani Varanasi, Materials Science Division and Dr. Mark Spector, Office of Naval Research.

This MURI began in FY13 and was granted to a team led by Professor Roberto Myers of Ohio State University. The objectives of this project include understanding the structure-property relationships for coupling heat and spin current in various materials and synthesize magnetic materials with extraordinary and tunable thermal conductivity due to spins, understanding non-equilibrium phonon-magnon transport and the mechanisms behind Spin Seebeck Effect, and finally measuring and understanding phonon-magnon drag and phonon-electron drag in materials.

If successful, this project may lead to long-term applications such as temperature sensors, thermal spintronic devices, solid-state Spin Seebeck Effect -based power generators, thermal management in electronic and vehicular applications, and tunable thermal conductivity in materials via magnetic field, microwaves, and light.

Nanoscale Control, Computing, and Communication Far-from-Equilibrium

The MURI topic author and manager of this project is Dr. Samuel Stanton, Mechanical Sciences Division.

This MURI began in FY13 and was awarded to a team led by by Professor James Crutchfield of the University of California – Davis. The objective of this MURI is to develop fundamental understanding to enable new synthetic nanoscale systems capable of behaving as information engines, performing tasks that involve the manipulation of both information and energy. Ultimately, a unified framework for understanding, designing, and implementing information-processing engines will be developed by a team of experts in information processing by dynamical systems, nonequilibrium thermodynamics, control theory, and nanoscale devices to search for and articulate the basic principles underlying the manipulation of information and energy by synthetic nanoscale systems. Theoretical predictions will be empirically validated in experimental nanoscale devices.

This research will enable new capabilities to (1) quantify the intrinsic computation in nanoscale thermodynamic systems, (2) to produce a thermodynamic theory for control and optimization of out-of-equilibrium nanoscale processes, and (3) to accomplish experimental validation of the resulting thermodynamic principles of optimization and control of molecular agents. The results will provide a scientific foundation for future nanoscale devices with groundbreaking capabilities, ranging from efficient computation on microscopic substrates to the generation of directed motion. In the long term, this research may enable devices that can coordinate the molecular assembly of materials and novel substrates for information processing on radically smaller and faster scales. This research may lead to a new generation of faster, cheaper, and more energy efficient computing devices capable of manipulating large-scale, complex data structures, as well as self-organizing nanoscale motors capable of interfacing with the physical world with maximum power and efficiency.

This success supports these ARL Core Technical Competencies:

Propulsion Sciences

Computational Sciences

Non-Equilibrium Many-Body Dynamics

The MURI topic authors and co-managers of this project are Drs. Paul Baker and Dr. Marc Ulrich, Physics Division.

This MURI began in FY13 and was awarded to a team led by Professor Cheng Chin at the University of Chicago. The goal of this MURI is to study fundamental non-equilibrium dynamics using cold atoms in optical lattices.

Dynamics far from equilibrium is of great importance in many scientific fields, including materials science, condensed-matter physics, nonlinear optics, chemistry, biology, and biochemistry. Non-equilibrium dynamics recently has taken on significance in atomic physics, where new tools will enable breakthroughs. In particular, optical lattice emulation is allowing one to gain insight, and potentially solve, traditionally intractable problems, including those out of equilibrium. Breakthroughs in other disciplines are also enabling a new look at non-equilibrium. In materials science, a recent pump-probe

This success supports these ARL Core Technical Competencies:

Network and Information Sciences

Materials and Manufacturing Sciences

experiment enabled dynamical control of material properties.[8] Another example is in biochemistry, in determining the role that non-equilibrium phase transitions play in driven biochemical networks, e.g., canonical phosphorylation-dephosphorylation systems with feedback that exhibit bi-stability.[9-10] Despite the ubiquitous nature of non-equilibrium dynamics, little scientific progress has been made due to the many challenges, including the difficulty in finding many-body systems that remain far from equilibrium on experimentally accessible time scales.

The objective of this MURI project is to discover how many-body systems thermalize from non-equilibrium initial states, and explore the dynamics of far-from-equilibrium systems. Given that non-equilibrium dynamics plays an important role in many scientific and engineering areas, such as quantum sensing and metrology, atomtronics, and quantum chemistry, this research could ultimately lead to the development of dynamic materials, and devices for improved computation, precision measurement, and sensing.

[8]Goulielmakis E, Yakovlev VS, Cavalieri AL, et al. (2007). Attosecond control and measurement: lightwave electronics. Science. 317:769-775.

[9]Qian H. (2006). Open-system nonequilibrium steady state: statistical thermodynamics, fluctuations, and chemical oscillations. J. Phys. Chem. B. 110:15063-15074.

[10]Ge H and Qian H. (2011). Non-equilibrium phase transition in mesoscopic biochemical systems: from stochastic to nonlinear dynamics and beyond. J. R. Soc. Interface. 8:107-116.

Theory and Experiment of Cocrystals: Principles, Synthesis and Properties

The MURI topic authors and co-managers of this project are Dr. James Parker, Chemical Sciences Division and Dr. Chakrapani Varanasi, Materials Science Division.

This MURI began in FY13 and was awarded to a team led by Professor Adam Matzger of the University of Michigan – Ann Arbor. This MURI team is investigating molecular co-crystal formation and the implications for controlling solid-state behavior.

The largely untapped potential for creating new molecular crystals with optimal properties is just beginning to be realized in the form of molecular co-crystallization. Co-crystallization has the potential to impact the macro-scale performance of many materials, ranging from energetic materials, to pharmaceuticals, to non-linear optics. Unfortunately, the dynamics of molecular co-crystal formation is poorly understood. Molecular co-crystals contain two or more neutral molecular components that rely on non-covalent interactions to form a regular arrangement in the solid state. Co-crystals are a unique form of matter, and are not simply the result of mixing two solid phases. Organic binary co-crystals are the simplest type and often display dramatically different physical properties when compared with the pure 'parent' crystals. A significant amount of research on co-crystal design has been carried out by the pharmaceutical industry for the synthesis of pharmaceutical ingredients. However, co-crystal design has not been exploited in broader chemistry and materials science research areas. A recent breakthrough discovery demonstrates that co-crystallization can be used to generate novel solid forms of energetic materials.

The objective of this MURI is to develop a fundamental understanding of intermolecular interactions in the context of crystal packing, and to use the knowledge gained for the design of new co-crystalline molecular materials with targeted, optimized physical and chemical properties. In the long term, a better understanding and control of molecular co-crystallization has the potential to improve the properties of a variety of materials, including: energetic materials, pharmaceuticals, organic semiconductors, ferroelectrics, and non-linear optical materials.

This success supports these ARL Core Technical Competencies:

Propulsion Sciences

Ballistics Sciences

Materials and Manufacturing Sciences

Chapter 06

Broad Agency Announcement FY19 Archive Excerpts

ARO is closely involved in writing or contributing to a wide range of Broad Agency Announcements (BAAs) across DoD and the Army. However, the chief BAA used by ARO to complete its mission is often referred to as the ARO Core BAA. The ARO BAA is open for submissions at any time throughout the year.

The publicly-available ARO Core BAA as of the final day of FY19 was W911NF-17-S-0002-05 (i.e., Modification 5 of the FY17-FY22 BAA with eligible submission dates 1 April 2017 – 31 March 2022).

This chapter provides key excerpts of the ARO Core BAA: Section II-A (Program Descriptions), which describes the research interests of ARO Programs in FY19.

This background image is from "3D-Printed Shape-Shifting Soft Robots that can Crawl, Jump and Grab" on page 271.

II. DETAILED INFORMATION ABOUT THE FUNDING OPPORTUNITY

A. Program Description

1. RESEARCH INTERESTS FOR U.S. INSTITUTIONS

ARL's ARO mission is to serve as the Army's principal extramural basic research agency funding research at universities, companies and not-for- profits in the engineering, physical, and information sciences. ARO's research portfolio is executed through ten scientific divisions, with titles reflecting fundamental scientific disciplines familiar to academic institutions. These Divisions directly support the ARL Core Technical Competencies. Additional information about the ARL S&T Core Technical Competencies can be found at the ARL website: www.arl.army.mil.

a. Physical Sciences

Research in the Physical Sciences is focused on basic research to discover, understand, and exploit physical, chemical, and biological phenomena. This research is of a fundamental nature; however, in the long term, discoveries in this area are expected to lead to revolutionary new capabilities in warfighter performance, intelligence, synthetic biology, sensing, communications, protection, power/energy storage and generation, and materials that extend the performance of Army systems well beyond current limits.

i. Chemical Sciences

The objective of the Chemical Sciences Division is to uncover and exploit the fundamental properties and processes governing molecules and their interactions in materials and chemical systems. The Division encourages proposals that promote basic research to develop methods for accurately predicting the pathways, intermediates, and energy transfer of specific reactions, to understand the fundamental processes governing electrochemical reactions and transport of species, and to discover the relationships between macromolecular microstructure, architecture, functionality, and macroscopic properties. In addition, these efforts will likely lead to new methods for synthesizing and analyzing molecules and materials that will open the door to future studies not feasible with current approaches.

The Division's research programs are currently focused on five research areas that include one program focused on international research. The titles, scopes and points of contact for these programs, each of which address general aspects of basic research in chemical sciences, are listed in the following subsections. Symposia, conferences and workshops are also supported in part or in whole to provide an exchange of ideas in areas of Army interest.

(1) Polymer Chemistry

The goal of this Program is to understand the molecular-level link between polymer microstructure, architecture, functionality, and the ensuing macroscopic properties.

Research in this Program may ultimately enable the design and synthesis of functional polymeric materials that give the Soldier new and improved protective and sensing capabilities as well as capabilities not yet imagined. This Program is divided into two research thrusts: (i) *Precision Polymeric Materials* and (ii) *Complex Adaptive Polymeric Systems*. Within these thrusts, high-risk, high-payoff research is identified and supported to pursue the Program's long-term goal.

The *Precision Polymeric Materials* thrust supports research aimed at developing new approaches for synthesizing polymers with precisely-defined molecular weight, microstructure, architecture, and functional group location. Of particular interest are research efforts that focus on novel methods for achieving sequence and tacticity control in synthetic polymers as well as enabling the synthesis of novel 2D organic polymers. Also of interest to this thrust are research efforts that explore how molecular structure influences polymer assembly into more complex, hierarchical structures as well as influence interactions with other materials (e.g., inorganic or biological materials) to render functional hybrid assemblies.

The *Complex Adaptive Polymeric Systems* thrust focuses on developing polymers that exhibit programmed molecular responses to external stimuli. Particularly of interest are research efforts related to stimuli-responsive self-immolative polymers, polymer mechanochemistry, and stimuli-mediated polymer assembly. Additionally, research focused on exploring the assembly/incorporation of multiple responsive groups into a single polymeric material system as well as the incorporation of feedback mechanisms to engender complex responsive behavior is also of interest.

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(2) Electrochemistry

This Program supports fundamental electrochemical studies to understand and control the physics and chemistry that govern electrochemical redox reactions and transport of species, and how these are coupled with electrode, catalysis, electrolyte, and interface. Research includes ionic conduction in electrolytes, electrocatalysis, interfacial electron transfer, transport through coatings, surface films and polymer electrolytes, activation of carbon-hydrogen and carbon-carbon bonds, and spectroscopic techniques that selectively probe electrode surfaces and electrode-electrolyte interfaces. Novel electrochemical synthesis, investigations into the effect of microenvironment on chemical reactivity, quantitative models of electrochemical systems, and electrochemistry using excited electrons are also of interest.

This Program is divided into two research thrusts, although other areas of electrochemical research may be considered: (i) Reduction-oxidation (Redox) Chemistry and Electrocatalysis, and (ii) Transport of Electroactive Species.

The *Redox Chemistry and Electrocatalysis* thrust supports research to understand how material and morphology affect electron transfer and electrocatalysis, to tailor electrodes

and electrocatalysts at a molecular level, and to discover new spectroscopic and electrochemical techniques for probing surfaces and selected species on those surfaces.

The *Transport of Electroactive Species* thrust supports research to uncover the mechanisms of transport through heterogeneous, charged environments such as polymers and electrolytes, to design tailorable electrolytes based on new polymers and ionic liquids, and to explore new methodologies and computational approaches to study the selective transport of species in charged environments.

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(3) Molecular Structure and Dynamics

The goal of the Molecular Structure and Dynamics program is to determine the reactive pathways and intermediates for reactions of molecules and molecular ions in gas and condensed phases at a range of temperatures and pressures, and to develop theories that are capable of accurately and efficiently describing and predicting these phenomena. In the long term, these studies may serve as the basis for the design of future propellants, explosives, and sensors. This Program is divided into three research thrusts: (i) *Reaction Dynamics*, (ii) *Computational Modeling*, and (iii) *Chemistry of Novel Energetic Materials*.

Research in the *Reaction Dynamics* thrust explores energy transfer mechanisms in molecular systems. In particular, research is focused on understanding dynamic processes such as roaming radicals, chemical reactions in solid state crystals and heterogeneous mixtures, phase transformations, kinetically stabilized versus thermally stabilized polymorphs and opportunities for control of polymorphic phase, and control of chemical processes using a variety of spectroscopic methods. Studies that yield new insights on the decomposition pathways of energetic molecules including their associated ionic states, both in the gas and condensed phases, are also of interest. The role that cations and anions play during detonation of bulk phase energetic materials is currently of high interest in the program. Proposals are especially encouraged in this area.

Research in the *Computational Modeling* thrust is focused on the development and validation of theories for describing and predicting the properties of chemical reactions and molecular phenomena in gas and condensed phases. In particular, research targeted at the development and implementation of novel theoretical computational chemistry methods is of interest. Ideally, such methods will go beyond current theories to allow for efficient, accurate, and *a priori* prediction of thermochemical properties. Such methods may take advantage of near-ideal parallel processing on massive computer clusters, or they may seek to solve current scaling problems through novel implementation of unprecedented theories via computer algorithms. The accurate prediction of intermolecular forces for problems in solid-state chemistry, such as the prediction of x-ray crystal structures, is also of interest.

Research in the *Chemistry of Novel Energetic Materials* thrust is focused on the synthesis, characterization, and measurement of properties of novel disruptive energetic materials. For a programmatic definition, disruptive energetic materials are those which have the potential to release two to ten times the explosive power of RDX when detonated. Such novel disruptive energetic materials will likely be derived from systems which differ significantly from traditional hydrogen-carbon-nitrogen-oxygen energetic materials. To be practical, any useful EM must have a high potential energy stored within the chemical bonds and also be stable from unwanted stimulations leading to accidental detonation. This principle can be used to develop notional disruptive energetic materials, and the methods of chemical synthesis can be used to target them for development. Academic research in this area is focused on discovery and characterization.

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(4) Reactive Chemical Systems

The goal of the Reactive Chemical Systems Program is to achieve a molecular level understanding of interfacial activity and dynamic nanostructured and self-assembled chemical systems to provide unprecedented hazardous materials management capabilities and soldier survivability. This Program supports basic research with Army relevance in surfaces, catalysis, organized assemblies, and stimuli-responsive chemical systems. This program is divided into two thrusts: (i) *Interfacial Activity* and (ii) *Synthetic Molecular Systems*.

The *Interfacial Activity* thrust supports research on understanding the kinetics and mechanisms of reactions occurring at surfaces and interfaces and the development of new methods to achieve precise control over the structure and function of chemical and biological molecules on surfaces. Specific areas of interest include adsorption, desorption, and the catalytic processes occurring at surfaces and interfaces and the interface between nanostructures and biomolecules to generate advanced materials.

The *Synthetic Molecular Synthesis* thrust supports research that imparts multi-functionality, stimuli-responsive and dynamic behavior to completely synthetic molecular and chemical systems. Research of interest includes design and development of nanostructured scaffolds and sequential catalytic systems. This thrust also supports research aimed at exploring the properties and capabilities of self-assembled and supramolecular structures, including their functionality, and how to control assembly in different environments.

In addition, the emerging field of dynamic, responsive, multi-functional materials have great potential to provide revolutionary new capabilities. A specific technical area in this field is "targeting and triggering" in which a specific chemical (or event) is targeted (recognized) and that recognition triggers a response. Particular technical challenges of interest include selective and reversible recognition, amplification, and multi-responsive

systems. Alternative approaches to selective, yet reversible, recognition are needed. Amplification includes an understanding of how to amplify the response from a single molecular recognition event to a multi-molecular response with approaches that promote chain reactions, self-amplification or cascade-type reactions within a single system. Multi-responsive systems in which specific stimuli trigger distinct responses are also of interest.

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(5) Energy Transport and Storage (International Program)

As one of the ARO International Programs, the Energy Transport and Storage Program is focused on supporting research at institutions outside of the U.S., with the goal of building international partnerships and laying the foundational work upon which future energy storage and power generation technologies depend.

Refer to Section II.A.2 of this BAA for a detailed description of this international research program's research goals, including the titles, scopes and points of contact for these programs.

ii. Physics

The objective of the Physics Division is to develop forefront concepts and approaches, particularly exploiting quantum phenomena, that will in the long-term have revolutionary consequences for Army capabilities, while in the nearer-term providing for existing Army needs. In support of this goal, the interests of the Physics Division are primarily in the areas described in the following subsections.

The Division's research programs are currently focused on five research areas, including one program focused on international research. The titles, scopes and points of contact for these programs, each of which address general aspects of basic research in physics, are listed in the following subsections. A small number of symposia, conferences and workshops are also supported in part or in whole to provide an exchange of ideas in areas of Army interest.

(1) Condensed Matter Physics (CMP)

The CMP Program strives to drive research that looks beyond the current understanding of natural and designed condensed matter, to lay a foundation for revolutionary technology development for next generation and future generations of warfighters.

Strong Correlations and Novel Quantum Phases of Matter. Understanding, predicting, and experimentally demonstrating novel phases of matter in strongly correlated systems will lay a foundation for new technology paradigms for applications ranging from information processing to sensing to novel functional materials. Interest primarily involves strong correlations of electrons, but those of other particles or excitations are

not excluded. This thrust also emphasizes dynamically- stabilized electronic states and metastable phases that are not adiabatically accessible from known ground states. The Program seeks to foster novel experimental and theoretical research targeting the discovery and rational design of new quantum phases of matter, along with exploring how excitations within these phases can be probed and controlled.

Topologically Non-Trivial Phases in Condensed Matter. Topologically non-trivial states of matter beyond the quantum Hall phases have shown a remarkable opportunity to advance our understanding physics as well as provide a foundation for new technologies. This thrust seeks to expand our understanding of both single-particle mean field topological states and those with strong correlations. Discovery as well as engineering of new non-trivial phases, verification of non-trivial topologies and phase transitions between trivial and non-trivial topological states and among the latter are of interest.

Unique Instrumentation Development. Advanced studies of CMP phenomena often require unique experimental techniques with tools that are not readily available. For example, unambiguous experimental verification of predicted topologically non-trivial phases can be beyond the reach of existing techniques. The construction and demonstration of new methods for probing and controlling unique quantum phenomena is of particular interest.

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(2) Quantum Information Science

Quantum mechanics provides the opportunity to perform highly non-classical operations that can result in beyond-classical capabilities in imaging, sensing and precision measurements, exponential speed-ups in computation, or networking. This Program seeks to understand, control, and exploit such non- classical phenomena for revolutionary advances beyond those possible with classical systems. An overarching interest is the exploration of small systems involving small numbers of entangled particles. There are three major areas of interest (thrusts) within this Program.

Foundational Quantum Physics (FQP). Experimental investigations of a fundamental nature of quantum phenomena, potentially useful for quantum information science, are of interest. Examples include coherence properties, decoherence mechanisms, decoherence mitigation, entanglement creation and measurement, nondestructive measurement, complex quantum state manipulation, and quantum feedback. An important objective is to ascertain the limits of our ability to create, control, and utilize quantum information in multiple quantum entities in the presence of noise. Systematic materials focused research which identifies and/or mitigates decoherence mechanisms is also of interest. Models of machine learning that are based on the foundations of quantum physics are of interest. Theoretical analyses of non-classical phenomena may also be of interest if the work is strongly coupled to a specific experimental investigation, such as proof-of-concept demonstrations in atomic, molecular, and optical (AMO) as well as other systems.

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Quantum Sensing, Imaging, and Metrology (QSIM). This research area seeks to explore, develop, and demonstrate multi-particle coherent systems to enable beyond classical capabilities in imaging, sensing, and metrology. Central to this research area is the exploration of small systems involving a few entangled particles. Topics of interest in this research area include the discovery and exploration of (a) multi-particle quantum states advantageous for imaging, sensing, and metrology, (b) quantum circuits that operate on multi-particle quantum states to enable beyond- classical capabilities, and (c) methods for the readout of quantum states. Other research topics of interest are: theory to explore multi-particle quantum states useful for beyond classical capabilities, quantitative assessment of capabilities and comparison to classical systems, efficient state preparation, quantum circuits for processing these states as quantum bits, readout techniques, decoherence mitigation and error-correction for improved performance, supporting algorithms as a basis for processing circuits, connections between the solution of hard computational problems and overcoming classical limitations in imaging, sensing, and metrology, entanglement as a resource, and suitable physical systems and key demonstration experiments.

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Quantum Computation and Quantum Networking (QCON). Quantum computing and networking will entail the control and manipulation of quantum bits with high fidelity. The objective is the experimental demonstration of quantum logic performed on several quantum bits operating simultaneously, which would represent a significant advance toward that ultimate goal of beyond classical capabilities in information processing. Demonstrations of quantum feedback and error correction for multiple quantum bit systems are also of interest. There is particular interest in developing quantum computation algorithms that efficiently solve classically hard problems, and are useful for applications involving resource optimization, imaging, and the simulation of complex physical systems. Examples include machine learning, parameter estimation, constrained optimization, and quantum chemistry, among others. The ability to transmit information through quantum entanglement distributed between spatially-separated quantum entities has opened the possibility for new approaches to information processing. Exploration of quantum networking of information and distributed quantum information processing based on entanglement is of interest. These include the exploration of long-range quantum entanglement, entanglement transfer among different quantum systems, and long-term quantum memory.

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(3) Atomic and Molecular Physics (AMP)

Topics of interest within the AMP Program include (i) quantum degenerate atomic gases, both Bose and Fermi, their excitations and properties, including mixed species,

mixed state, and molecular, (ii) quantum enhanced precision metrology, (iii) nonlinear atomic and molecular processes, (iv) quantum topological matter, (v) collective and many-body states of matter, and (vi) emerging areas. Cooling schemes for molecules are of importance for extending the range of systems that may be exploited. In addition, there is an interest in emerging areas of AMO physics such as states of topologically protected matter including but not limited to topological phases, emergent lattices in quantum gases, opto- mechanical interfaces, non-equilibrium many body dynamics, and many-body localization. Research efforts within the AMP Program fall within two thrust areas: *Advanced Quantum Capabilities* and *Novel Quantum Methods*. It is anticipated that research efforts within these areas will lead to applications including novel materials, efficient computational platforms, and exquisite quantum sensors.

Advanced Quantum Many-body Dynamics. The focus of this thrust is the development and study of strongly interacting many-body systems. The quantum simulator portion of the thrust seeks research on novel cooling, trapping, and the expansion of atomic and molecular species. The effort seeks the validation of many-body quantum theories through the development of experimental tools including quantum gas microscopes, synthetic gauge fields, mixed species, and novel interactions. Complimenting this effort will be the inclusion of foundational investigations into quantum mechanics, such as entanglement, many-body localization, topologically protected states, and entropy. To take advantage of the precision inherent in future quantum devices, these systems will need to connect to the classical world in such a manner that allows them to sample the signal of interest while remaining robust to noisy environments. Investigating how to maximize both the quality and quantity of entanglement within these systems will be a priority. General issues of quantum coherence, quantum interference, entanglement growth, entanglement purity, and non-equilibrium phenomena, as well as discovering new scientific opportunities are also of interest.

Novel Quantum Metrology. The AMP Program has a general interest in exploring fundamental AMP that may impact future Army capabilities. This thrust is divided into two main areas: precision metrology beyond the standard limit and harnessing collective many-body states to improve quantum sensing. The Novel Quantum Metrology efforts will expand the foundations of quantum measurement into new areas that seek to exploit entanglement, spin-squeezing, harnessing collective-spin state, developing back-action avoidance measurements, and other areas that increase fundamental precision through interactions, including cavities and Rydberg atoms. It is expected that research in this thrust will complement efforts in the *Advanced Quantum Many-body Dynamics* thrust and *vice versa*. For example, collective many body states could be studied in optical lattices or quantum gas microscopes and foundational research of entanglement and topologically protected states are anticipated to provide new metrological capabilities.

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(4) Optical Physics and Fields

The objective of this Program is to investigate physical phenomena that will lead to a deeper understanding of the underlying physics or the discovery of new physical effects that can improve capabilities of the Army. In particular, this program emphasizes physics that will significantly improve areas such as remote sensing, information processing, light and energy transmission, interactions between light and matter, and new or emerging phenomena relating to optical physics and fields. Much of the Army's capability in sensing and information and/or energy exchange depends on light. This Program also seeks research for other long-range physical fields that can complement electromagnetic radiation.

Extreme Light. This thrust focuses on research on extreme light, meaning the examination of light in the extreme limits, such as the shortest pulses attainable and the highest intensity fields attainable. Advances in these areas require theoretical and experimental research. For example, ultrashort pulsed lasers have now achieved intensities of 10^{22} W/cm^2. Future applications of these pulses may include high-harmonic generation, nanolithography, particle beam acceleration and control, and light filaments. In addition, effects such as THz formation and control and broadband localized radiation from filaments are of interest. In the near future, even higher intensities are expected. Theoretical and experimental research efforts are needed to describe and understand how matter behaves under these conditions—from single particle motion and radiation reaction to the effects in materials—and how to generate these pulses and use them effectively. Pulses as short as 80 attoseconds have been produced, and the Program seeks ways to make them shorter and to understand both the physics and applications of this form of radiation. Proposals for new areas of extreme light such as relativistic optics are welcome.

Meta-Optics. This thrust pursues a fresh start in optics due to the new kinds of effects allowed by optical metamaterials. In this area, many conventional limits of optics can be broken in ways such as sub-wavelength imaging and superlensing related phenomena. It is timely to look at the quantum optics of such processes as well as research in in flat photonics. Proposals for new areas involving discrete symmetries, such as parity-time symmetries and non-Hermitian Hamiltonians are of interest. A related area is supersymmetric optics (SO), where project are sought that use SO concepts in the design of photonic materials with nee properties or capabilities. New forms of imaging using transformation optics or other novel imaging, including quantum optics, are also of interest. In general, any optical phenomena that can ultimately improve Army capabilities are sought.

Non-Electromagnetic Fields. Other forms of propagating energy have been predicted and will theoretically have properties that differ dramatically from electromagnetism. Modern theories of gravity as well as string theory predict, in addition to gravity, the existence of two other long- range fields. If these theories are correct in their predictions, this suggests applications in which these new fields may be useful for detection or communication, especially in situations where electromagnetism and optics are not useful, such as propagating through conducting media. This program seeks proposals that may lead to the detection and/or measurement of these fields.

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(5) Quantum Scale Materials (International Program)

As one of the ARO International Programs, the Quantum Scale Materials Program is focused on supporting research at universities outside of the U.S., with the goal of providing key connections with world-class researchers outside the U.S. and supporting the most forward-looking physics research.

Refer to Section II.A.2 of this BAA for a detailed description of this international research program's research goals, including the titles, scopes and points of contact for these programs.

iii. Life Sciences

The Life Sciences Division supports basic research to advance scientific knowledge and understanding of the fundamental properties, principles, and processes governing DNA, RNA, proteins, organelles, prokaryotes, and eukaryotes, as well as multi-species communities, biofilms, individual humans, and groups of humans. Research investments are driven by exploiting new scientific opportunities with anticipated long-term payoffs, including maintaining U.S. technological superiority and developing new Army capabilities.

The interests of the Life Sciences Division are primarily in the following areas: synthetic biology, biochemistry, neuroscience, microbiology, molecular biology, genetics, genomics, proteomics, epigenetics, systems biology, bioinformatics, and social science. The results of fundamental research supported by this Division are expected to enable the creation of new technologies for improving warfighters' physical and cognitive performance capabilities, for protecting warfighters, to create new human-machine synergistic capabilities for identifying causes of and tipping points for social/political instability, and for creating new Army capabilities in the areas of biomaterials, energy, logistics, forensics and intelligence.

The Division's research programs are currently focused on seven research areas, which includes two programs focused on international research. The titles, scopes and points of contact for these programs, each of which address general aspects of basic research in life sciences, are listed in the following subsections. A small number of symposia, conferences and workshops are also supported in part or in whole to provide an exchange of ideas in areas of Army interest.

(1) Biochemistry

This Program emphasizes basic research focused on understanding and controlling the activity and assembly of biomolecules. Scientific advances supported by this Program are anticipated to enable the development of novel systems, materials and processes that

enhance Soldier protection and performance. An overarching goal of the Program is to provide the scientific foundations to support biological activity outside of the cellular environment, including integration of biological systems with synthetic systems.

The *Biomolecular Specificity and Regulation* thrust is focused on elucidating natural mechanisms by which biomolecules recognize and interact with their targets, as well as inherent regulatory mechanisms utilized to activate or inhibit biomolecular activity. This research thrust also includes novel approaches to engineer the specificity and regulation of biomolecules, either via modulation of natural mechanisms or via design of non-natural mechanisms. The goal of this thrust is to develop novel engineered approaches to modulate and control biomolecular activity, with emphasis on achieving biomolecular control in non-cellular contexts.

The *Biomolecular Assembly and Organization* thrust is focused on understanding the molecular interactions and design rules that govern self-assembly of biomolecules into both naturally occurring biomolecular structures and non-natural human-designed architectures. Biomolecular assembly across length scales is of interest, including discrete multi-protein complexes or nucleic acid structures, as well as hierarchical protein or nucleic acid assemblies and biological composites. This thrust includes homogeneous assemblies utilizing a single building block, as well as heterogeneous systems in which a mixture of different biomolecules and/or non-biological species (e.g., minerals, synthetic polymers) assemble. This thrust aims to elucidate fundamental understanding of sequence-structure-property relationships in natural biomolecular assemblies, biomaterials, and biological composites to enable rational design of biological and hybrid biological/abiological assemblies with tailored properties and/or functions. This research thrust also includes the design of self-assembled biomolecular or hybrid biological/abiological architectures that support functional organization of biological molecules in non-cellular contexts, including artificial cells and cell-free systems, as well as novel approaches to achieve functional integration of biomolecules with non-biological materials.

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(2) Genetics

This Program supports basic research in genetics, molecular biology, genomics, epigenetics, and systems biology in areas that may enable the optimization of the Soldier's cognitive and physical performance capabilities, increase Soldier survivability, and improve Army capabilities in areas such as biomaterials, sensing, energy, and intelligence. This Program emphasizes innovative high-risk fundamental research in areas such as identification and characterization of gene function, gene regulation, genetic interactions, gene pathways, gene expression patterns, epigenetics, mitochondrial regulation and biogenesis, and nuclear and mitochondrial DNA replication, mutagenesis, oxidative stress, and DNA repair.

The *Eukaryotic Genetics, Genomics, Epigenetics and Molecular Biology* thrust is

focused on identifying and characterizing genes, genetic pathways and genetic regulation in eukaryotes. This Program is interested in identifying and understanding the molecular factors and genetic polymorphisms that affect human physical and cognitive performance capabilities as well as human survival and protection under normal conditions and when affected by a variety of stressors likely to be encountered in battlefield situations, such as dehydration, heat, cold, sleep deprivation, fatigue, caloric insufficiency, pathogens, and physical and psychological stress. This program is also interested in pollen and species distribution models, mitochondrial regulation, activity and integrity, nuclear and mitochondrial DNA stability and instability, alternative animal systems, social insects, biological components of social instability, trust, plant genetics, synthetic biology, endosymbionts, and biological systems for sensing and detecting.

The *Prokaryotic Genetics, Genomics, Epigenetics and Molecular Biology* thrust is focused on understanding prokaryotic genes, genomes, molecular biology and epigenetics. Areas of interest include mechanisms of prokaryotic adaptation at a molecular, individual and population level, prokaryotic genetic stability and instability, and synthetic biology.

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(3) Microbiology

This Program supports basic research in fundamental microbiology that can help advance needs in Soldier protection and performance. There are two primary research thrusts within this program: (i) Prokaryotic Survival Mechanisms in Challenging and Extreme Environments and (ii) Analysis and Engineering of Microbial Communities.

The *Prokaryotic Survival Mechanisms in Challenging and Extreme Environments* thrust focuses on the study of the cellular and genetic mechanisms and responses that underlie not just microbial survival in the face of environmental stress, but also the ability of specific microbes to thrive under those conditions. These stressors include extremes in temperature, pH, or salinity; the presence of toxins including metals and toxic organic molecules; oxidative stress; and cellular starvation and the depletion of specific nutrients. Included here is the study of microbial metabolism under conditions of slow growth and the transitions into and out of slow growth phases. Research approaches can include fundamental studies of microbial physiology and metabolism, cell biology, and molecular genetics that examine key cellular networks linked to survival and environmental adaptation, microbial cell membrane structure and the dissection of relevant critical signal transduction pathways and other sense-and-respond mechanisms.

The *Analysis and Engineering of Microbial Communities* thrust supports basic research that addresses the fundamental principles that drive the formation, proliferation, sustenance and robustness of microbial communities through reductionist, systems-level, ecological and evolutionary approaches. Bottom-up analysis of nutrient consumption, information exchange, signaling interactions, spatial/temporal effects structurefunction relationships and biosynthetic output for single and multi-species communities within

the context of planktonic and both native and engineered biofilm architectures is considered. The use of these approaches for the analysis of model microbial systems that address the biology of the mammalian microbiome are welcome. Of joint interest with the ARO Biomathematics Program, research efforts that advance the ability to work with complex biological data sets to increase understanding of microbiological systems marked by ever-increasing complexity are encouraged.

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(4) Neurophysiology of Cognition

The Neurophysiology of Cognition program supports non-medically oriented basic research in neuroscience, the behavioral sciences, physiology and neuroengineering that might enable the optimization of Soldier's cognitive and physical performance capabilities. An overarching goal of the program is to provide foundational knowledge of molecular, cellular and systems-level neural codes underlying cognition and performance across multiple length and time scales. Research in this program can include a broad range of methodological and theoretical approaches applied to animal and human experimental systems including electrophysiology, neuroimaging and computational neurobiology. This includes the study of the psycho-physiological implications of brain-machine interfaces, the measurement and modeling of individual cognitive dynamics and decision making during real-world activity, and identifying how neuronal circuits generate desirable computations. In the long term, research in this area may enable the development of interfaces enabling humans to more efficiently control machines, new training methods and devices to predict and optimize individual performance, and the potential restoration from injury at the neural level. Basic research opportunities are sought in two primary research thrusts within this program: (i) Multisensory Synthesis and (ii) Neuronal Computation.

Multisensory Synthesis. The Multisensory Synthesis thrust aims to understand how the human brain functions in relation to the interaction of sensory, cognitive and motor processes during its performance of real-world tasks. Research focuses on mapping, quantifying and modeling distributed neural processes, physiological processes and mind-body interfaces that mediate these features to ultimately develop better understanding of cognition for eventual application to Soldier performance.

Neuronal Computation. The Neuronal Computation thrust is focused on understanding how living neuronal circuits generate desirable computations, affect how information is represented, show robustness to damage, incorporate learning and facilitate evolutionary change. Research focuses on determining how brains structure, process and refine inputs into efficient decisions and behaviors, and how these multiscale features are altered under stresses. Cell culture, brain slice and *in vivo* models are used to develop better understanding of small and large-scale living neural networks for eventual application in Army systems.

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(5) Social and Behavioral Science

The goal of this Program is to promote basic research on social behavior to discover the theoretical foundations of social behavior at all levels, from single agents to collectives and global societies. The thrusts of this Program are (1) developing reliable and valid measures and models of social and behavioral dynamics, (2) discovering, modeling, and validating theories of interactions among social, natural, and physical systems; and (3) generating new cross-cultural models of the impact of social institutions on the scientific enterprise.

Measuring & Modeling Social and Behavioral Dynamics. The behavior of single agents comprises a social system. The individual behaviors, however, cannot simply be summed to accurately depict or predict the dynamics of a social system. There are a number of well-documented intervening collective processes (e.g., polarization, evaluation apprehension, Ringlemann effect, risky-shift, information transfer biases, identity decay, risk transfer) that may lead to local or system-wide adjustments. Little is known about the conditions under which such collective processes are activated or how they interact to affect collective outcomes. Moreover, existing methods to detect them are often fraught with bias, relying on subjective self-reports, reliance on instruments that are not cross-culturally consistent, observer/experimenter bias, demand effects in experiments, and non-representative sampling frames. In addition to challenges in measuring social dynamics, traditional methods of modeling and empirically testing theoretical claims are often deficient. There is a tendency to use statistical techniques that rely on assumptions that are not borne out in the social phenomena being studied (e.g., assumptions of linear relationships, continuous scales, non-independence of observations, normally distributed data). The aim of this thrust is to inform and advance social science theories by generating and validate measures, methods, technologies, and models that objectively capture individual and collective dynamics to overcome this gap. The thrust looks favorably on the use of emerging methods in biophysiological measurements, measurement of social dynamics of non-human species, and cross-cultural research. It also encourages non-traditional modeling strategies that overcome deficiencies of using continuous linear models and normal distributions when phenomena are not continuous, linear, or normally distributed, as well as overcoming inappropriate assumptions of non-independence of observations. This thrust will enable new capabilities for the Army to more accurately predict risks posed by single agents, collectives, and regimes, as well as provide a foundation for understanding the basis for improving performance in and outcomes of collectives and populations.

Modeling and Validating Interactions among Social, Natural, and Physical Systems. Social systems are embedded in a larger ecological system consisting of turbulent and dynamic natural phenomena (e.g., droughts, floods, earthquakes) and constantly evolving physical systems (i.e., human-built systems, including dense urban environments, cyber environments, utility systems, transportation routes). This embeddedness imposes tensions on social systems, which may shift global social orders, impact alliances, incite conflicts, and generate sociopolitical instabilities. Different social systems, however, may be more or less resilient to the shifts in natural and

physical systems. While this is anecdotally recognized, rigorous research to model the interactions among these systems is relatively new and beset with methodological challenges arising from the difficulty of tracking impacts of one system on another over different temporal and spatial expanses, the multi-level character of how effects from one system spillover to another, a lack of ability to identify how features of one system impact features of another (e.g., how the physical infrastructure of a city impacts the resilience of the city to shocks from natural disasters). Capturing the fragility/resilience of social systems to shifts in natural and physical systems will enable improved capabilities to predict emerging regions of potential future social unrest and violence, providing the Army with an early warning system to forecast and prepare for emergent conflict and the ability to plan and mobilize multidomain operations.

Modeling the Scientific Enterprise. Science is an inherently social activity and while recent research has explored the social networks of science (e.g., who publishes with whom, who mentors whom) and the demographics of actors in those networks, there is very little rigorous research on the overall enterprise of science and the impact of social institutions, like economic, political, educational, and religious systems on the trajectory of science: what leads to a discovery; how do discoveries transition to application; why do some discoveries lie dormant for decades before an application is realized, while others are almost immediately translated to application. Taxonomies related to science have been developed for example to describe (a) categories of science (e.g., Pasteur's Quadrant), (b) relations between funding and scientific activities in the research and development pathway (e.g., 6.1 – 6.7), (c) pathways from basic science to obsolescence (e.g., "cradle-to-grave"), (d) types of research strategies (e.g., "exploration vs. exploitation"),and (e) changing states of discoveries (e.g., "Sleeping Beauty Effect"). But these are merely systems of categorization and fail to capture the dynamic and socially embedded nature of science that leads to scientific discovery and leads scientific discovery to transition from one state to another. There is a long history in the philosophy of science that does recognize the social dynamics of science, but has yet to be operationalized. Organizational science has developed case studies of organizations that rapidly generate discoveries and transition them to swiftly seize market dominance. While rich in description, case studies fall short of a generalizable theory of the scientific enterprise. The aim of this thrust is to pursue new models that capture the socially embedded dynamic nature of science by focusing on science not as only a local team-driven or organizationally specific phenomena, but also investigate science as a macro institutionally motivated enterprise. A macro perspective on science will provide new insights on factors that enable both discovery and inventions that improve lives and capabilities. This thrust encourages formal modeling strategies using cross-cultural data to depict the impact of culturally unique configurations of social processes and institutions that affect science, discovery, and transitions. Success in this thrust will result in new insights on how social institutions catalyze and impede science.

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(6) Synthetic Biology (International Program)

As one of the ARO International Programs, the Synthetic Biology Program is focused on supporting research at institutions outside of the U.S., with the goal of providing key connections with world-class researchers outside the U.S. and supporting the most forward-looking studies in synthetic biology.

Refer to Section II.A.2 of this BAA for a detailed description of this international research program's research goals, including the titles, scopes and points of contact for these programs.

(7) Human Dimension (International Program)

As one of the ARO International Programs, the Human Dimension Program is focused on supporting research at institutions outside of the U.S., with the goal of providing key connections with world-class researchers outside the U.S. and supporting the most forward-looking research in this area.

Refer to Section II.A.2 of this BAA for a detailed description of this international research program's research goals, including the titles, scopes and points of contact for these programs.

b. Engineering Sciences

Research in the Engineering Sciences is focused on basic research to discover, understand, and exploit new material systems, mechanical systems, electronics, and earth sciences that are expected to create revolutionary capabilities for the Army. Discoveries in this area are expected to lead to capabilities in materials, the sciences for propulsion, the information domain, the ballistics sciences, the protection sciences, and human sciences augmentation, well beyond the limits facing today's Army.

i. Mechanical Sciences

The Mechanical Sciences Division supports research in a broad spectrum of fundamental investigations in the disciplines of fluid dynamics, solid mechanics, complex dynamics and systems, and propulsion and energetics. Though many creative and imaginative studies concentrate on a particular sub-discipline, increasingly, new contributions arise from interdisciplinary approaches such as the coupling between aerodynamics and structures, complex dynamics and systems, combustion and fluid dynamics, or solid mechanics and structures as in the structural reliability areas. Additionally, several common themes run through much of these four sub-disciplines, for example, active controls and computational mechanics. Research in such areas is addressed within the context of the application rather than as a separate subject of study. Fluid dynamics research is primarily concerned with investigations in the areas of rotorcraft wakes, unsteady aerodynamics of dynamic stall and unsteady separation, and fundamental studies of micro adaptive flow control. Solid mechanics include a wide array of research areas such as high strain rate phenomena, penetration mechanics, heterogeneous material behavior, and reliability of structures. The complex dynamics and systems area is focused on investigations in vehicle structural dynamics, and

simulation and air vehicle dynamics including rotor aeromechanics. Research in the propulsion and energetics area is concentrated on processes characteristic of reciprocating (diesel) and gas turbine engines and the combustion dynamics of propellants used for gun and missile propulsion. The following narratives describe the details of the scope and emphasis in each of these sub disciplinary areas.

The Division also supports the ARL S&T Core Technical Capabilities. This includes the Propulsion Sciences through research in hydrocarbon combustion, non-equilibrium dynamical systems, unsteady separation and dynamics stall, and vortex dominated flows S&T areas, and the Protection Sciences and Ballistics Sciences through research in energetics, multi-scale mechanics of heterogeneous solids, and low-stiffness, nonlinear materials and material systems S&T areas. These efforts also contribute to lesser extent to the Materials & Manufacturing Sciences and Human Sciences Competencies through its impacted S&T areas.

The Division's research programs are currently focused on four research areas. The titles, scopes and points of contact for these programs, each of which address general aspects of basic research in mechanical sciences, are listed in the following subsections. Symposia, conferences and workshops are also supported in part or in whole to provide an exchange of ideas in areas of Army interest.

(1) Fluid Dynamics

Fluid dynamics plays a critical role in many Army operational capabilities. Significant challenges exist for accurate and efficient prediction of flow physics critical for improved performance and future advanced capability. Army platforms are often dominated by flows with high degrees of unsteadiness, turbulence, multiple and widely separated spatio-temporal scales, and geometrical complexity of solid or flexible boundaries. In order to gain the necessary physical insight to enable future capabilities spanning Army vehicles, munitions, medical devices, and logistics, the Fluid Dynamics program seeks to support basic research investigations of fundamental and novel flow physics. In view of the nonlinear and high-dimensional character of the governing equations, revolutionary advances in fluid dynamics research tools are also of great interest; advanced experimental methods, sophisticated computational techniques and breakthrough theoretical advances will be critical for gaining the required fundamental understanding. There are three major subareas or thrusts within the Fluid Dynamics program: Dynamics of Unsteady and Separated Flows, Nonlinear Flow interactions and Turbulence, and Flow Stability and Control. Each of these is described in detail below.

Dynamics of Unsteady and Separated Flows. Operating conditions for many Army platforms are characterized by flows featuring unsteadiness, nonlinear interactions, turbulence, three-dimensionality and flow separation. All efforts in this thrust area will require novel and aggressive strategies for examination of the interplay between disparate spatio-temporal scales, inclusion of physically significant sources of three-dimensionality, and characterization of the role of flow instabilities and nonlinear interactions across a range of appropriate Mach and Reynolds numbers. Criteria for

identifying the signature of unsteady separation and/or incipient separation are of particular interest. Historical management of physical complexity has often resulted in scientific approaches that result in the elimination of potentially critical flow physics. Research efforts that are capable of gaining deep understanding of highly complicated flows are likely to allow critical physics to be exploited, leading to significant performance gains for Army systems. As an example, shortcomings in understanding the details of unsteady flow separation, reverse flow phenomena, and dynamic stall continue to limit the capabilities of Army rotorcraft vehicle platforms. While much progress has been made towards unraveling these details, it has become apparent that revolutionary advances are unlikely if the full complexity of the physics is not considered.

Nonlinear Flow Interactions and Turbulence. As mentioned above, many Army relevant flows are governed by strong nonlinearities and turbulent behaviors. Historically, many analysis tools developed for linear dynamics have been applied to gain understanding of flow behaviors. While local insights can be gained through applications of these methods, the ability to provide global understanding of the evolution of flows requires new approaches that are capable of dealing directly with inherent nonlinearities. Operator theoretic methods show great promise in tackling the perennial difficulties associated with the Navier-Stokes equations. Turbulent dynamics may also benefit from new approaches based in dynamical systems theory to push modeling frameworks beyond the notions based on Reynolds averaging and stochastic dynamics and to determine if a useful underlying deterministic structure exists. Modeling flows near walls is a continuing challenge to accurate numerical prediction of complex physics that may benefit from novel non-intrusive diagnostics to inform creative numerical and theoretical constructs capable of efficiently producing a high degree of fidelity near physical boundaries.

Flow Stability and Control. Many of the previously described flows are susceptible to initially small amplitude, but dynamically significant, instabilities that can ultimately lead to fundamental changes in global flow behaviors. Thorough understanding and prediction of these instabilities and their growth is crucial not only to maintaining robustness in the face of disturbances, but also to gain advanced control over the evolution of flows through their exploitation. Research breakthroughs in global and local stability characteristics and their subsequent manipulation are of interest. Theoretical, computational, and experimental examinations of canonical problems to enable focused studies of interactions between instability mechanisms and global flow characteristics are highly encouraged, especially those that seek nonlinear descriptions. Flow control efforts should seek to exploit understanding of these mechanisms to permit the flow evolution to be prescribed. Flow control investigations should also seek to understand not only the impact of control actuation on the flow, but should also consider strategies for closed-loop feedback control and appropriate scaling laws that lead to the potential for such strategies to transition into new capabilities in real-world flows.

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(2) Solid Mechanics

The goal of the Solid Mechanics Program is to investigate and understand behavior of complex material systems a under broad range of loading regimes in various environments and to develop analytical and computational methods to characterize material models which can serve as physically-based tools for the quantitative prediction and control of Army relevant material systems subjected to extreme high loading and strain rate conditions such as impact and blast. The program seeks novel approaches to innovate unprecedented systems and structures with previously unattainable properties and behaviors. Research in analytical, computational and experimental solid mechanics is sought to form the foundation for understanding these systems as well as to validate developed physical models. Understanding of failure in soft and active material systems is also of interest to the program. Such work should lead to novel ideas and concepts for revolutionary capabilities.

The understanding of the mechanics of material behavior during transition into states of damage and fracture initiation due to extreme loading, high rate loading, high-temperature variations, and repetitive loading are of interest. The program seeks the development of models of material behavior across broad spatial and temporal scales that are based on these physical processes taking place at different scales and of establishing essential physical understanding of the relationships of the various processes taking place such that failure may be accurately predicted.

Novel experimental methods aimed to investigate and validate material models play on all scales are sought. Development of new experimental techniques is essential for solid mechanics development. In particular, the program seeks techniques to enhance the understanding of the physical processes taking place during deformation and failure in the interior of materials.

Computationally efficient methods capable of integrating the new physical relationships and models, and with the ability to predict the behavior of novel material systems in extreme conditions across a broad range of scales are sought.

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(3) Complex Dynamics and Systems

The Complex Dynamics and Systems Program emphasizes fundamental understanding of the dynamics, both physical and information theoretic, of nonlinear and nonconservative systems as well as innovative scientific approaches for engineering and exploiting nonlinear and nonequilibrium physical and information theoretic dynamics for a broad range of future capabilities (e.g. novel energetic and entropic transduction, agile motion, and force generation). The program seeks to understand how information, momentum, energy, and entropy is directed, flows, and transforms in nonlinear systems

due to interactions with the system's surroundings or within the system itself. Research efforts are not solely limited to descriptive understanding, however. Central to the mission of the program is the additional emphasis on pushing beyond descriptive understanding toward engineering and exploiting time-varying interactions, fluctuations, inertial dynamics, phase space structures, modal interplay and other nonlinearity in novel ways to enable the generation of useful work, agile motion, and engineered energetic and entropic transformations. Further information on the current scientific thrust areas are detailed in the paragraphs that follow.

High-Dimensional Nonlinear Dynamics. Classical dynamics has produced limited fundamental insight and theoretical methods concerning strongly nonlinear, high-dimensional, dissipative, and time-varying systems. For over a century, qualitative geometric approaches in low-dimensions have dominated research in dynamics. These approaches of reduced-order-modeling of high-dimensional dynamics are often premised on empirical and statistical model fitting and are incapable of capturing the effects of slowly growing instabilities and memory. The program seeks to develop novel theoretical and experimental methods for understanding the physical and information dynamics of driven dissipative continuous systems. It also seeks novel reduced-order-modeling methodologies capable of retaining time-dependent and global nonlinearities. Novel research pertaining to the analysis and fundamental physics of time-varying nonlinear systems and transient dynamics is a high-priority.

Nonlinear Mechanical Metastructures. Another emerging area in this thrust concerns nonlinear mechanical metastructures. Emphasis is on exploiting nonlinear behavior within nonlinear mechanical lattices and lattices of nonlinear mechanical modules from the millimeter to meter scale. Proposals exploring interactions between nonlinear meta-structures with fluids, especially if such interactions augment desired dynamic behavior, are strongly encouraged.

Embodied and Distributed Control, Sensing, and Actuation. This thrust develops deeper understanding, through supporting theory and experiment, of the role of embodiment and dynamics on a physical system's capability to process information and transform energy. Proposals emphasizing the mechanics and control of soft, continuous bodies are encouraged along with novel experimental paradigms leveraging programmable printed matter. Generally, this thrust strongly leverages advances in, and approaches from, sensory biomechanics, neuromechanics, underactuated systems theory, and mechanical locomotion dynamics to understand the motion of both articulated and continuum dynamical systems operating in highly-dynamic environments. The scientific principles sought, however, are not limited to biological movement and manipulation. Proposals are strongly encouraged that view morphology in an abstract sense. For example, understanding morphology as a system's symmetry, its confinement (e.g. chemical reactions), or its coupling topology.

Statistical Physics of Control and Learning. The program seeks to lay the foundations for an algorithmic theory of control and learning that goes significantly beyond the state-of-the-art in model predictive control and integrates novel learning methodologies that

are not mere variations of artificial neural networks and deep learning. Additional goals of this program is to develop an experimentally tested theoretical framework for controlling and creating new types of critical dynamics, phase transitions, and universality classes by bringing together theory and physical principles in statistical dynamics with control and dynamical systems theory (controlling statistical dynamics). Topics of interest relating to this include: nonlinear control of distributions with non-Gaussian uncertainty; non-Gaussian uncertainty representations; understanding relationships between work absorption and dynamics in the presence of fluctuations leading to emergent prediction and emergent centralization; steering multi-critical interacting dynamical systems toward desired universal scaling behaviors; externally controlling the strength of stochastic fluctuations and intrinsic noise in systems that are driven far from thermal equilibrium and display generic scale invariance; and selectively targeting and stabilizing specific self-generated spatio-temporal patterns in strongly fluctuating reaction-diffusion systems. Stochastic control at the microscale to enable novel manipulation of the dynamics of synthetic and natural biomolecular machines is also of interest.

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(4) Propulsion and Energetics

Propulsion and Energetics Research supports the Army's need for higher performance propulsion systems. Future systems must provide reduced logistics burden (lower fuel/propellant usage) and safer (insensitive) higher energy density systems. Fundamental to this area are the extraction of stored chemical energy and the conversion of that energy into useful work for vehicle and projectile propulsion. In view of the high temperature and pressure environments encountered in these combustion systems, it is important to advance current understanding of fundamental processes to enable truly predictive models as well as to advance the ability to make accurate, detailed measurements for the understanding of the dominant physical processes. Thus, research in this area is characterized by a focus on high pressure, high temperature combustion processes and on the peculiarities of combustion behavior in systems of Army interest.

Hydrocarbon Combustion. Research on combustion phenomena relevant to diesel cycle engines is focused on intermittent reacting flows containing fuel injection processes, jet break-up, atomization and spray dynamics, ignition, and subsequent heterogeneous flame propagation.as well. Gaining fundamental understanding of these phenomena pertaining is a major objective. Novel diagnostics for the investigation of the dense field region of the spray are of special interest. Research on heterogeneous flames requires supporting study into kinetic and fluid dynamic models, turbulent flame structure, soot formation and destruction, flame extinction, surface reactions, multiphase heat transfer, and other factors that are critical to an understanding of engine performance and efficiency. An additional consideration is the high pressure/low temperature ignition environment encountered in advanced engines, which influences liquid behavior and combustion processes at near-critical and super-critical conditions.

Fundamental research is needed in many areas, including low temperature physical and chemical rate processes, combustion instability effects at low temperatures, and non-equilibrium behavior. New characterization methods to investigate kinetics and flame phenomena in-situ at high pressure are needed. New computational methods to be able to predictively model complex reacting systems are also needed. With advances in sensing, modeling, and control architectures, it is becoming possible to further optimize the performance of combustion systems. Providing the foundations for such active control is also of interest to the program.

Energetic Materials. Research on energetic material combustion processes is focused on understanding the dynamics of the planned and inadvertent ignition and subsequent combustion of these materials which are commonly used for propulsion in gun and missile systems and in ordinance. The program is also addressing the characterization of advanced energetic materials, e.g., those based on nanoscale structures and/or ingredients. Basic research is needed in several areas, including: thermal pyrolysis of basic ingredients and solid propellants; flame spreading over unburned surfaces (particularly in narrow channels); surface reaction zone structure of burning propellants; chemical kinetics and burning mechanisms; propellant flame structures; characterization of physical and chemical properties of propellants and their pyrolysis products; and coupling effects among the ignition, combustion, and mechanical deformation/fracture processes. The use of advanced combustion diagnostic techniques for reaction front measurements, flame structure characterization, and determination of reaction mechanisms is highly encouraged, especially those able to probe surface and sub-surface reactions in the condensed phase. Also of interest are novel methods which can well characterize the ignition and burning behavior of a material utilizing only minute quantities of that material. Complementary model development and numerical solution of these same ignition and combustion processes are also essential. There is also need to understand the unplanned or accidental ignition of energetic materials due to stimuli such as electrostatic discharge, impact, friction, etc. This requires, for example, research on the processes of energy absorption and energy partitioning in the materials, the effect of mechanical damage on the ignition events, and other topics relating to the safety of energetic materials.

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ii. Electronics

The Electronics Division seeks to support scientific and engineering endeavors in research areas that possess the potential to define new electronic capabilities or to enhance future electronic performance. The Division is more concerned with generating basic knowledge about processes and mechanisms than creating actual devices, although prototype devices may be useful for demonstration of principle. The Electronic research sub-areas are (1) Nano and Bio- Electronics, (2) Optoelectronics, (3) Electronic Sensing, and (4) Electromagnetics and High Frequency Electronics. Proposals are sought that advance fundamental understanding of electronic and photonic processes leading to new or improved materials and devices with a strong prospect for use in future Army technology.

The Electronics Division supports many of the ARL S&T Competencies especially the Materials & Manufacturing Sciences which is supported by all Electronics' sub-areas in novel electronic and photonic materials. The Computational Sciences Competency is supported through novel Nano, Bio, and Optoelectronic computing, Protection Sciences by active and passive sensing, Network & Information Sciences by new algorithms from biosciences as well as electromagnetic discoveries, Ballistics Sciences and Protection Sciences through targeting and directed energy, and Human Sciences through understanding and interfacing electronically with biological systems.

The Division's research programs are currently focused on four research areas. The titles, scopes and points of contact for these programs, each of which address general aspects of basic research in electronics, are listed in the following subsections. Symposia, conferences and workshops are also supported in part or in whole to provide an exchange of ideas in areas of Army interest.

(1) Biotronics

This research area focuses on the discovery and manipulation of phenomena and the creation of new processes where electronics and biology overlap at the cellular / sub-cellular level. This length scale is where the amplitudes of many types of energies (e.g., electrostatic, mechanical, and chemical terms) converge, and correspondingly, where electronics can have fundamental biological impacts and where leveraging electronics capabilities at the nanoscale can yield unique new understanding of the cellular and intracellular processes. New electronic structures and materials are now able to focus localized static electric and magnetic fields and electromagnetic fields at the nanoscale, which presents the opportunity to selectively address and manipulate the organelles and membranes making up the structure of the cell. Moreover, cell constituents can have a frequency dependent response to mechanical and electromagnetic excitation, resulting in unique electronically enabled and controlled biological experiments. Molecular and subcellular events at the biological interfaces or surfaces are key to downstream biological dynamics. The stimulation or manipulation of these events by electronic means provides the opportunity for unique control and experimentation that are orthogonal to existing biochemical or genetic approaches. Ion flow, which is fundamental to inter- and intra-cellular signaling and process control, is susceptible to electromagnetic influence and produces electromagnetic signatures of cellular processes. The dynamics of charged and polarized cellular components also produces minute displacement currents, and can produce very large field distributions in a confined nanoscale space (e.g., within a protein scaffold or across a lipid bilayer); both of which are subject to electromagnetic probing and analysis. The different geometries of organelles within a cell result in different electromagnetic signatures and sensitivities which can be leveraged for selective control of cellular processes. Proteins play a role in almost every cellular process. As extremely large and complex molecules, they should have electromagnetic and mechanical responses that can be exploited for control. The skeletal protein assemblies of the cell, in particular, may offer a highway for the introduction of electrical currents or mechanical vibrations. Bio-chemical or genetic

alteration of the interface of the cell and its components can introduce new electromagnetic properties, for example a new capability for photosynthesis in bacteria or new electromagnetic responses. Cellular engineering of membranes, cellular organelles, and proteins by the introduction of nano-particles and bio-molecules can introduce new sensitivities and new functionality. Opto-genetics is a well-established procedure for interrogating cells. Early attempts at "magneto-genetics" have been controversial, however "electro- or RF-genetics" may offer new opportunities. There may also be inherently non-trivial quantum mechanical mechanisms linked to biological behaviors, such as navigation. Inherently quantum phenomena such as the tunneling of electrons and protons play a critical role in many intracellular processes and can be modulated or manipulated with nanoscale electric fields. This research area seeks understanding and control of inter- and intra-cellular phenomena at the micro- and nano-scale.

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(2) Optoelectronics

Research in this subarea includes novel semiconductor structures, processing techniques, and integrated optical components. The generation, guidance and control of UV through infrared signals in semiconductor, dielectric, and metallic materials are of interest. The Army has semiconductor laser research opportunities based on low dimensional semiconductor structures (quantum dots, wells, wires, etc.) operating in the eye-safe (>1.55), 3-5, 8-12, and 18-24 microns regions for various applications, such as ladar, infrared countermeasures, and free space/integrated data links. Components and sources in the UV/visible spectral ranges (particularly < 300 nm) may be of interest as well. Research is necessary in semiconductor materials growth and device processing to improve the efficiency and reliability of the output of devices at these wavelengths.

Research that leads to an increase in the data rate of optoelectronic structures is sought. Interfacing of optoelectronic devices with electronic processors will be investigated for full utilization of available bandwidth. Electro-optic components will be studied for use in guided wave data links for interconnections and optoelectronic integration, all requirements for high speed full situational awareness. Optical interconnect components are needed in guided-wave data links for computer interconnection and in free-space links for optical switching and processing. For high-speed optical signal processing as well as potential for power scaling, research on individual and 1 or 2-D arrays of surface or edge-emitting lasers is necessary. Research addressing efficient, novel optical components for high speed switching based on plasmonics, quantum dots, metamaterials or other regimes may be of interest. Emitters and architectures for novel display and processing of battlefield imagery are important.

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(3) Electronic Sensing

The ultimate goal of Army sensing is 100% situational awareness to include day/night, all weather, non-line-of-sight and through natural and man-made obstructions for sensing of vehicles, personnel, weapons, chemical and biological threats, projectiles, explosives, landmines, improvised explosive devices (IEDs), and motion. Novel techniques that enhance the stimulus-response characteristics of nano-structures and semiconductor devices are of interest. This includes ways to improve the absorption of the signal, conversion (transduction) of the signal to another form with higher efficiency, and techniques to lower the noise. Sensing technologies of interest to this research sub- area currently include acoustic; seismic; passive electromagnetic; magnetic, and light-matter interactions. Other technologies that meet an Army need are also welcome, however chemical, biological, and radar sensing techniques are generally funded through other sub-areas as is image processing.

Light-matter interactions at infrared and ultra-violet wavelengths are of particular interest. Efforts are sought that improve the quantum efficiency and lower the noise such that the signal to noise ratio is maintained as the temperature is increased. Research opportunities include components based on quantum confined devices and semiconductor materials operating in the infrared 1-24 microns regions as well as the ultra-violet spectral region. In both regions, fundamental studies involving growth, defects, interfaces, substrates, doping, and other electronic characteristics will be considered. Back-of-the-envelope calculations of the detectivity or noise equivalent power should be included for proposals involving infrared and ultra-violet detection.

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(4) Solid State and Electromagnetics

This research area emphasizes efforts to discover and create unique electromagnetic phenomena in solid-state materials and structures. Innovative research is sought in areas involving quantum phenomena, internally and externally induced stimulus, and novel transport and electromagnetic interaction effects in solid-state electronic structures. This basic research will address issues related to design, modeling, fabrication, testing and characterization to include the ability to individually address, control, and modify structures, materials and devices, and the assembly of such structures with atomic-scale control into systems. It will seek realize advanced device concepts with revolutionary capabilities.

This program will explore the latest developments in semiconductor materials and device physics, such as negative capacitance transistors, tunneling field effect transistors and ultra-wide bandgap materials. More importantly, it will emphasize scientific discoveries in the frontier of nanoelectronic materials and structures. Scientific opportunities in this research include, but are not limited to, quantum-confined structures (nano-tubes/-wires/-dots) and large- scale precise alignment and integration of these structures to create collective behaviors; 2D atomic crystals and their heterostructures; complex heterostructures of 2D crystals, topological insulators, Dirac and Wely semimetals and other dissimilar nanoelectronic materials potentially leading to unique

interfacial phenomena; spintronic, valleytronic, and mixed domain (charge/spin/quantum degrees of freedom) device concepts. Of interest are quantum transport phenomena such as ballistic transport and hydrodynamic flow, dissipationless transport in topologically protected edge states, and pseudo-relativistic transport of massless Dirac fermions. Exotic electromagnetic phenomena which require theoretical formulations beyond the well-established Maxwell's equations, such as axion electrodynamics, chiral anomaly and spontaneous symmetry breaking, are also relevant. Interfacial proximity effects in these heterostructures that lead to unique electromagnetic properties will also be considered.

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iii. Materials Science

The Materials Science Division of the ARO seeks to realize unprecedented material properties by embracing long-term, high risk, high-payoff opportunities for the US Army with special emphasis on: Materials Design, Mechanical Behavior of Materials, Physical Properties of Materials, and Synthesis and Processing of Materials. Research supported by the Division seeks to discover the fundamental relationships that link chemical composition, microstructure, and processing history with the resultant material properties and behavior. The work, although basic in nature, is focused on developing new materials, material processes, and properties that promise to significantly improve the performance, increase the reliability, or reduce the cost of future Army systems. Fundamental research that lays the foundation for the design and manufacture of multi-component and complex materials is of particular interest. Foundational research that integrates novel experimental work with the development of new predictive materials theory is also of significant interest. Furthermore, there is lasting interest in new ideas and cross-disciplinary concepts in materials science that may have future applications for the Army.

The Division supports the ARL Materials & Manufacturing Sciences Competency by aggressively seeking to extend the state-of-the-art in materials design, mechanical behavior of materials, physical properties of materials, and synthesis and processing research. It further accomplishes this with unique materials for advanced power storage and generation and lightweight structures, in addition to low-cost manufacturing and repair processes. It supports the ARL Ballistics Sciences with extraordinary lightweight materials, force-activated materials, stabilized nanostructured materials, manufacturing process science, novel electronics, and advanced sensory materials. It also supports the ARL Computational Sciences with research efforts that integrate computational theory and precision experimental measurement to design and optimize advanced materials.

The Division's research programs are currently focused on five research areas that include one program focused on international research. The titles, scopes and points of contact for these programs, each of which address general aspects of basic research in materials science, are listed in the following subsections. Symposia, conferences and workshops are also supported in part or in whole to provide an exchange of ideas in areas of Army interest.

(1) Materials Design

The Materials Design program seeks to establish the experimental techniques and theoretical foundations needed to facilitate the hierarchical design and bottom-up assembly of multifunctional materials that will enable the implementation of advanced materials concepts including transformational optics, biomimetics and smart materials.

Directed 3D Self-Assembly of Materials is aimed at enabling the directed 3D assembly of reconfigurable materials, and developing viable approaches for the design and synthesis of multi-component materials incorporating hierarchical constructs and tolerant of structural defects.

Functional Integration of Materials focuses on demonstrating the predictive design and integration of functional properties and feedback control into complex multi-component systems, and developing analytical techniques for interrogating the evolution of the 3D structure and properties of material assemblies at the nanoscale.

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(2) Mechanical Behavior of Materials

The Mechanical Behavior of Materials program seeks to reveal underlying design principles and exploit emerging force-activated phenomena in a wide range of advanced materials to demonstrate unprecedented mechanical properties and complementary behaviors.

Force-Activated Materials focuses on the creation, design, and optimization of a broad range of robust mechanochemically adaptive materials, based on exquisite control of force-activated molecules and force-activated reactions, and on tailoring the deformation and failure mechanisms in materials to mitigate the propagation of intense stress-waves and control energy dissipation.

Mechanical Complements in Materials endeavors to create materials with the ability to facilitate extraordinary electrochemical reactions through an interdependent optimization of mechanical properties, to catalyze the discovery and demonstration of unique fiber precursors, tailored for lateral and axial interactions, toward new paradigms for revolutionary structural fibers, and to discover and optimize new atomic-scale strengthening mechanisms governing bulk mechanical behavior.

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(3) Physical Properties of Materials

The Physical Properties of Materials program seeks to elucidate fundamental mechanisms responsible for achieving extraordinary electronic, photonic/optical,

magnetic and thermal properties in advanced materials to enable innovative future Army applications.

Novel Functional Materials supports the discovery of novel functional materials such as free-standing 2D materials/heterostructures/hybrids, Spin-Caloritronic materials, co-crystals, and other such materials with unique structures/compositions. The thrust focus is on the synthesis, modeling and novel characterization of these materials (organic/inorganic/hybrids) to determine unprecedented functional properties (semiconducting, superconducting, ferroelectric/multiferroic etc.).

Science & Engineering of Crystal Imperfections explores the influence (either positive or negative) of various crystal imperfections (e.g. point, line, area, volume defects etc.) on the physical properties of functional materials, and elucidates different mechanisms of incorporation during thin film growth/bulk materials processing of materials to influence the resulting extraordinary functional properties.

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(4) Synthesis and Processing of Materials

The Synthesis and Processing of Materials program seeks to discover and illuminate the governing processing-microstructure-property relationships to enable optimal design and fabrication of nano or micro structural bulk structural materials.

Processing Induced Material Design supports research focused on innovative processing methods capable of fabricating materials with deliberate microstructural architectures and features that advance the material's properties to levels unattainable by conventional processing.

Manufacturing Process Science supports investigation into fundamental physical laws and the unique phenomena occurring under metastable and far-from-equilibrium conditions to develop revolutionary and disruptive new materials or processing methodologies.

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(5) Innovations in Materials (International Program)

As one of the ARO International Programs, the Innovations in Materials Program is focused on supporting research at institutions outside of the U.S., with the goal of building international partnerships and laying the foundational work upon which future material technologies depend.

Refer to Section II.A.2 of this BAA for a detailed description of this international research program's research goals, including the titles, scopes and points of contact for these programs.

iv. Earth Sciences

The Earth Sciences Division of the ARO seeks to advance understanding of the terrestrial environment for the U.S. Army with special emphasis on Earth Materials and Processes and Environmental Chemistry. Research supported by the Division seeks to explore the properties of Earth materials and chemical species to discover how they interact with their environments and respond to external forces. Knowledge of the fundamental properties of these materials, from the atomistic to the landscape scale, and their interactions with the atmosphere, hydrosphere, and biosphere are relevant to Army operations, infrastructure, and stewardship. Fundamental research lays the foundation to support a range of Army needs, including the remote characterization of land surfaces, trafficability of ground vehicles, and environmental priorities such as waste management and remediation. Furthermore, there is lasting interest in new ideas and cross-disciplinary concepts in Earth science that may have future applications for the Army.

The Division's research programs are currently focused on two research areas. The titles, scopes and points of contact for these programs, each of which address general aspects of basic research in earth sciences, are listed in the following subsections. Symposia, conferences and workshops are also supported in part or in whole to provide an exchange of ideas in areas of Army interest.

(1) Earth Materials and Processes

The Earth Materials and Processes program seeks to elucidate the properties of natural and man-made Earth surfaces, with the goals of revealing their histories and governing dynamics and developing theory that describes physical processes responsible for shaping their features.

Earth Surface Materials aims to utilize experiments, models, and theory development to describe the physical and mechanical properties and behaviors of rocks, minerals, and soil, and to exploit the properties of these materials to provide quantitative information on recent and ongoing surface processes and perturbations.

Surface Energy Budget aims to determine, at Army-relevant spatial and temporal scales, how natural and artificial surfaces (e.g., soil, sand, or concrete) store and conduct energy depending on their spatial relationships, inherent material properties, and imparted features such as moisture storage and evapotranspiration, and to determine how these surfaces affect flows in complex terrain.

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(2) Environmental Chemistry

The goal of the Environmental Chemistry program is to understand the fate and transport

of chemicals that in the long term will enable future force protection, and water treatment. This program seeks to encourage research to provide a more complete and practical understanding of chemical pathways of degradation and transformation in the environment. The research will embrace environmental complexity by including the study of multiple phases and chemicals simultaneously present. Environmental surfaces of interest are soils (e.g., clay, sediments, dust), water (e.g., surface and bulk, snow and ice structures) and films (e.g., biological and urban made). The program will identify fundamental research opportunities in two main thrusts: (i) *Chemical Fate and Transport*, and (ii) *Environmental Forensics*.

The *Chemical Fate and Transport* thrust interest is in mechanisms, thermodynamics and kinetics with a focus on experimental and theoretical approaches to investigate sorption, degradation, and photo degradation mechanisms of chemical species under environmentally relevant conditions. Of particular interest is understanding the conditions that lead to degradation and transformation of contaminants, and develop novel speciation models of complex environmental media.

The *Environmental Forensics* thrust focuses on developing integrated experimental and computational approaches to discern chemical transformation of contaminants from source to point-of-detection and provide predictions of its future transformations in different environments and conditions. In addition, this thrust includes research to provide information about manufacturing process and location of chemicals released into the environment.

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c. Information Sciences

Research in the Information Sciences is focused on discovering, understanding, and exploiting the mathematical, computational, and algorithmic foundations that are expected to create revolutionary capabilities for the future Army. Discoveries in this area are expected to lead to capabilities in materials, the information domain, and Soldier performance augmentation, well beyond the limits facing today's Army.

i. Computing Sciences

The principal objective of the ARO Computing Science Division is to provide increased performance and capability for processing signals and data, and to extract critical information and actionable intelligence to enhance the warfighters' situation awareness, decision making, command and control, and weapons systems performance. The Division supports research efforts to advance the Army and nation's knowledge and understanding of the fundamental principles and theories governing intelligent and trusted computing. More specifically, the Division aims to promote basic research to establish new computing architectures and models for intelligent computing, create novel data fusion and extraction techniques for efficient information processing, and build resilient computing systems for mission assurance. The results of these research efforts will stimulate future research and help to keep the U.S. at the

forefront in computing sciences. The research topics described in this section of the BAA are those needed to provide the warfighters with the latest information science and technology to achieve the vision of future Army operations.

Research in the Computing Sciences Division will reveal previously unexplored avenues for new Army capabilities while also providing fundamental results to support ARL's (i) Network & Information Sciences Competency goal of algorithm design for object classification and scene understanding from active and passive 3D scenes and full motion video through enhanced semantic object recognition; (ii) Computational Sciences goal of large scale computing and modeling, and dynamic multi-dimensional heterogeneous data analytics, by devising scalable algorithms that effectively handle the size, complexity, heterogeneity, and multi-modality of data and by creating new hardware and software architectures for emerging and future computing systems that optimize the use of Army computational resources; and (iii) the Network & Information Sciences Competency goal of estimating adversarial dynamics and infrastructure through new game models for capturing attacker/defender interactions and better predication of adversarial mental state (intent, capability, and decision process) to enable better cyber defense.

The Division's research areas are currently focused on five research areas that include one program focused on international research. The titles, scopes and points of contact for these programs, each of which address general aspects of basic research in computing science, are listed in the following subsections. A small number of symposia, conferences and workshops are also supported in part or in whole to provide an exchange of ideas in areas of Army interest.

(1) Computational Architectures and Visualization

The Computational Architectures and Visualization program is concerned with modeling, analysis, design, and validation of computational infrastructure, both hardware and software, with special emphasis on the effect emerging and future computational architectures will have on managing, processing, analyzing, and visualizing massive data sets. This is due to the fact that the Army's ability to generate data of all types from the battlefield to the laboratory far outpaces the Army's ability to efficiently manage, process, analyze, and visualize such massive amounts of information. Emerging architectures only exacerbate the problem because the present and traditional models of computation no longer apply.

The research strategy is to focus on the effect that the technological shift to these new, advanced architectures will have on newly-developed systems and how to compute with these architectures efficiently as well as to make very large simulations and the visualization of massive data sets more interactive for the user while maintaining a high level of accuracy. As such, this programs funds innovative architectural designs of both hardware and software components and their interfaces that efficiently optimize computational resources and innovative algorithms that render massive data sets and/or massive geometric models and perform large scale Army simulations both quickly and accurately. Advances in this program are expected to lead to new computer modeling and design concepts (or paradigms) as well as software libraries that compute efficiently

on these new and emerging architectures, that are scalable (usable on large-scale complex problems and able to handle massive amounts of data), and accurate (precise enough to predict and detect phenomena of interest) for both the laboratory and the battlefield. Also to be expected is the development of more efficient, interactive, and physically realistic battlefield, training, and scientific simulations.

Computational Architectures. Future computer systems will be both massively heterogeneous and parallel, implying the present and traditional models of computation will no longer be applicable. As a result, new computational theories are needed as well as mathematical abstractions and models of computation to address the difficulties associated with heterogeneous, parallel and distributed processing. Of special interest is determining how these new abstractions, algorithms, and computational processes map onto emerging computational resources of different types (e.g., multi-core, quantum, cloud, and chaotic computing, and determining which platforms are most suitable for Army applications). Other important issues to be considered for these emerging and future architectures are programmability, language and compiler support, real-time scheduling, resource-allocation, and the development of a flexible software environment.

Visualization. Interactive simulation and visualization provides new and enhanced capabilities for the examination, exploration, and analysis of information and data critical to the Army. However, Army applications are not limited to any one type of data or computational platform. As a result, new research and techniques are needed in order to visualize and simulate complex Army data such as training for battlefield scenarios with speed and precision on any platform for superior analysis and information extraction capabilities for realistic Army simulations and full situational awareness. Specific research areas of interest are, but not limited to, computational geometry, robust geometric computing, geometric and solid modeling, interactive graphics, 3D visualization tools, verification and validation, and synthetic environments. Special emphasis is placed on making very large simulations and the visualization of massive data sets faster, more computationally efficient, and more interactive for the user while maintaining an appropriate level of fidelity and physical realism.

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(2) Information Processing & Fusion

With ubiquitous data acquisition capabilities, effective data and information processing is of critical importance to defense missions. The Information Processing and Fusion program is concerned with the creation of innovative theories and algorithms for extracting actionable intelligence from diverse, distributed multimodal data to support Army operations.

Foundations of Image and Multimodal Data Analysis. Innovative research is sought concerning: (1) novel representations of multimodal data to enable the understanding of multimodal sensor data and contextual information, with particular emphasis on data in complex forms such as image or video data; (2) detection, localization, and recognition

of objects and locations from image data with particular emphasis on provable performance guarantees; (3) detection of events, actions, and activities to extract activity-based intelligence, especially when no extensive training data is available; and (4) integrated approaches that enable semantic descriptions of objects and events including relations. Learning and adaptation should enable the representation at both low and high-levels, where inputs from actual users of the systems are used to improve the performance of the algorithms and the fidelity of models at all levels of the modeling hierarchy. Also of interest are methods to exploit the structure of the data, capture its intrinsic dimensionality, and extract information content of data. The development of an "information/complexity theory" and a "learning theory" specific for remote sensing, imaging data, and decision tasks is highly desirable.

Data and Information Fusion. Multimodal data acquisition systems are increasingly prevalent with disparate sensors and other information sources. This thrust seeks advanced mathematical theories and approaches for integrating multimodal data and contextual information to provide actionable intelligence. Of particular interest are systematic and unifying approaches for data and information fusion from diverse sources. Scalable methods are needed for efficiently handling vast amounts of data. Fusion in networked environments addressing issues such as adaptive, distributed, and cooperative fusion is emphasized. Theories and principles for performance analysis and guarantees at all fusion levels to support robust data and information fusion are important to ensure successful military operations.

Active and Collaborative Sensing. Modern sensing systems typically include multiple networked sensors with communication capabilities where the whole network can be thought of as a Meta sensor that can be controlled, in addition to each individual node having some controllable degrees of freedom such as mobility for unmanned aerial/ground systems, pan-tilt-zoom for infrastructure sensors, or waveform for agile radar. Depending on the task or query, it is desirable for the system to control the data acquisition process so as to acquire the "most informative data" for the specific task or query. Consequently, of particular interest are methods that address the integration of mobility, sensor-selection, modality selection, and active observation for real-time assessment and improvements of sensing performance. Another research area of interest is performance-driven active data collection. A query is given to the system together with a desired performance bound. Where the confidence in answering the query is insufficient, the system should actively interrogate or control sensors in order to achieve the desired confidence. Such an active learning and information-driven sensor control should include the Soldier in the feedback loop.

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(3) Information and Software Assurance

From the Army perspective, Information Assurance must provide authentic, accurate, secure, reliable, timely information to warfighters in order to achieve information dominance, regardless of threat conditions. Computing and information processes may

be carried out over distributed and heterogeneous systems, which may include mobile computing and communications systems, and high performance information process systems that are inter-connected through both tactical and strategic communication systems.

Robust and Trusted Wireless Communication. Research is needed in the areas of theory, protocols, and techniques that will assure delivery of trustworthy data to support battlefield missions. Reconfigurable, survivable, and self-healing systems allow a combat unit to dynamically establish and maintain its command and communication capability under diversified and extreme battlefield situations. The Army requires a fully mobile, fully-communicating, agile, and situation-aware force that operates in a highly dynamic, network centric environment. This force consists of a heterogeneous mixture of individual soldiers, ground vehicles, airborne platforms, unmanned aerial vehicles (UAVs), robotics, and unattended sensor networks that operate in a complex wireless environment. Information theory has played a foundational role in the study of security. Across a wide range of application domains and security objectives, information theory leads to insight to the underlying tradeoffs between security and performance. The Army seeks novel ideas in fundamental research areas such as information-theoretic security and the science of security that will provide direct guidance in the design of secure tactical wireless systems. In particular, topics of interest include new paradigms for physical layer security (ranging from confidentiality to authentication to trustworthiness in physical layer communications), the fundamental bounds in key management in distributed systems, the exploitation of key establishment and distribution protocols, and trusted information delivery and dissemination in mobile environments. The corresponding constructions that would arise from such an investigation represents a significant avenue for improving future wireless communication as well as the corresponding secrecy capacity limits that could serve as valuable guidelines in developing future systems with confidential and authenticated communications. New computing and communication protocols and techniques are needed to assure critical information processing and delivery even when such systems are under severe resource constraints or under persistent attacks.

Models and Metrics for Next Generation Survivable Systems. The field of information assurance needs a foundational science to guide the design of systems and to quantitatively measure safety and the level of assurance of complex systems that the Soldier depends upon today. Assurance principles and metrics are needed to help define, develop, and evaluate future robust and resilient systems and network architectures that would survive sophisticated attacks and intrusions with measurable confidence. The program seeks the capability to measure a complex system and to produce a scalar value that can determine the trustworthiness of that system. In addition, human users need to be in the loop for system assurance analysis. Developing human centric security-usability metrics, computational models for usable security in stressful situations, and adaptive security protocols according to perceived threats are some of the research areas of interest for improving warfighter performance while maintaining sufficient security requirements. One new challenging area of research that offers great promise in stronger system robustness is the modeling of adversaries and defender interactions, since

ultimately systems need to defend effectively against their attacks. A deeper understanding and more accurate modeling of adversarial behaviors will improve future system development.

Cyber Deception. Cyber deception is a proactive technique to manipulate the mental state and decision process of the adversary so that we can degrade and mitigate their attack effectiveness. Unique aspects of cyber deception may offer more opportunities but add more complexity to model and analyze: 1) Cyber artifacts (both genuine and fake) can be created easily and are not bounded by the laws of physical space. The velocity of cyber situation change could be very high; 2) while deceptions are normally played out between a defender and an attacker, users could be directly or indirectly entangled in the game due to the nature of shared infrastructure. Usability issues or negative impact to the mission need to be considered; 3) Social and cultural aspects are important elements in the cyber deception game. Key scientific understanding is still lacking in 1) Establishing effective mental models for understanding and tracking the adversaries' intent, capability, and decision process, and 2) deception information formulation and communication techniques, which requires new thinking in order to provide a quantifiable measure on how a given deception approach will drive metal state change. Recent honeypots/decoy experiences gave initial insights on how to engage adversaries through fake cyber artifacts, but a clear understanding of the dynamics (especially mental interactions) between attackers and defenders is missing. A better learned adversarial model will be critical to the success of cyber deception. In addition, advanced honeypot like schemes are desired to engage adversaries in order to gain understanding of adversaries so that effective deception schemes can be crafted.

Principles of Moving Target Defense. Current cyber defenses are often static and governed by lengthy processes, while adversaries can plan their attacks carefully over time and launch the attacks at cyber speeds at times of their choosing. The program seeks a new class of defensive strategies to present adversaries with a moving target where the attack surface of a system keeps changing. Although such an idea of a "moving target" is a powerful paradigm for building systems robust to security threats, many fundamental aspects associated with such a strategy need to be further investigated and understood. For example, such a "moving target" system may operate under many different contexts, ranging from the use of frequency hopping in spread spectrum to software diversification. It is critical to establish new theories and models that can provide trade-off analysis between system robustness against attacks vs. performance/usability, and quantify the risks associated with system adaptation under an adversarial setting. Ultimately the understandings and analytical models obtained will establish an important foundation for creating robust tactical systems capable of maximizing the difficulties for the adversaries to attack while minimizing the impact to system performance and usability.

Trusted learning for cyber autonomy. Given a massive amount of data coupled with strong computation power, machine learning (ML) algorithms such as deep neural networks have shown initial success in many applications. However, without considering an adversarial setting, studies have shown fatal vulnerabilities in current AI

systems where a small adversarial perturbation can easily fool current AI into making wrong decision. The main contributing factors to AI vulnerability are: 1) the black box data driven approach provides no guarantee of either correctness nor security assurance; 2) current learning regime is extremely brittle since it assume that both training testing data are from the same stationary i.i.d. distributions commonly violated in real world, especially under an adversarial setting; 3) given an ultra-high dimensional data space, blind data spots do exist from training and can be easily exploited by adversaries. Given the serious adversarial risks to ML based systems, it is critical to carefully re-examine and rethink the fundamental aspects of ML that leads to its brittleness. It is critical to study and establish adversarial models which is the most critical first step in defense so that both correctness and robustness in learning and decision making for cyber defense can then be quantified. New scientific understandings are sought in terms of attack resilient learning, decision making and cyber autonomy, both at the data driven layer and the knowledge layer so that cyber defense relying on learning and adaptation will be more robust and resilient against adversarial manipulation and exploits.

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(4) Intelligent Systems

Computational intelligence is becoming an important part of our life and plays a critical role in defending the nation, both in physical and cyber space. Advanced capability in learning, understanding, reasoning, and decision making are key elements of intelligent systems. However, compared to humans, machine intelligence is still at its infancy. Important issues such as robustness, adaptability, awareness, and realism are the frontier of research today. Advances in these areas will contribute to the development of intelligent systems that can greatly enhance the Army's capabilities in mobility, agility, lethality, and survivability.

Advanced Learning Theory, Methodology, and Techniques. Machine learning to build computational intelligence has been studied for the past 50 years. While great strides have been made in artificial intelligence as demonstrated by the success of Deep Blue and recently AlphaGo, compared to biological systems, machine learning still lacks the rigor, agility, and adaptation and is quite fragile to changing environment or context. This thrust focuses on establishing a theoretical foundation of machine learning. New learning approaches will need to address both the dimensionality challenges and temporal characteristics that may be evolving continuously. In addition, new techniques must address robustness where the learning system will be able to deal with incorrect input due to noise and observation errors and potentially malicious input that aims to disrupt learning. Adaptation in learning is another major challenge. It is critical to create an advanced system that can continuously learn and evolve to changing context and environment, update its knowledge base accordingly, and dynamically adapt its reasoning, decision, and action.

Intelligent Systems for Improved Decision Making. Intelligent systems span a wide

spectrum of applications, from autonomous robotics such as Unmanned Ground Vehicle (UGV) and UAV to software decision making tools for Command, Control, Communications, Computers, Intelligence, Surveillance, and Reconnaissance (C4ISR). Quite often intelligence systems are engaged in sensing, perception, reasoning and understanding, learning, collaboration, and taking actions in an autonomous way. For these systems, sensing and vision understanding functions play a key role in establishing perception and situation awareness and help perform complex tasks such as navigation. Robust networking, communication and information processing ensure mission execution and contribute to a shared knowledge base, coordination and collaborations for dynamic environments. A common trait of intelligent systems lies in their capability in processing information along with suitable context and environment to make the best decisions and to take appropriate actions. An ideal intelligence system would have a strong cognitive capability that would enable itself to deal with environmental changes, to carry out new tasks, and cope with unknown situations. Unfortunately the current generation of intelligent systems have fairly narrow scopes and are designed to perform specific tasks, thus are quite often unable to adapt to a changing environment. New research is needed to create a new intelligent system with advanced cognitive capabilities that can successfully integrate advanced learning, knowledge representation and organization, cognitive reasoning, adaptation, and autonomous action.

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ii. Mathematical Sciences

The objective of the Mathematical Sciences Division is to support research to develop a foundational framework for the understanding and modeling of complex nonlinear systems, for stochastic networks and systems, for mechanistic models of adaptive biological systems and networks, and for a variety of partial differential equation (PDE) based phenomena in various media. These research areas focus on discovering nonlinear structures and metrics for modeling and studying complex systems, creating theory for the control of stochastic systems, spatial-temporal statistical inference, data classification and regression analysis, predicting and controlling biology through new hierarchical and adaptive models, enabling new capabilities through new bio-inspired techniques, creating new high-fidelity computational principles for sharp-interface flows, coefficient inverse problems, reduced-order methods, and computational linguistic models.

Research in the Mathematical Sciences Division will reveal previously unexplored avenues for new Army capabilities while also providing fundamental results to support ARL's (i) Information Sciences Competency goal of image and video sampling and reconstruction through investigations of sparsity in combinations of distributions with unknown parameters; (ii)
Computational Sciences Competency goals of stochastic simulation methods, interfaces and evolving topologies, and uncertainty propagation, through investigations of fast separable methods for stochastic PDEs, of novel meshes for both front tracking and domain-fitting, and of weak-interaction processes; (iii) Computational Sciences Competency goal of computational social sciences by establishing a general theory of crisis/change through new mathematical

models that go beyond network models to incorporate morphisms as model elements; (iv) Human Sciences Competency goals of brain networks and of cognitive and neural modeling, through investigations of neural dynamic models and their computation; and (v) Computational Sciences Competency goal of stochastic optimization and modeling through investigations of fast separable methods for stochastic PDEs.

The Division's research programs are currently focused on four research areas. The titles, scopes and points of contact for these programs, each of which address general aspects of basic research in mathematical science, are listed in the following subsections. A small number of symposia, conferences and workshops are also supported in part or in whole to provide an exchange of ideas in areas of Army interest.

(1) Modeling of Complex Systems

The Modeling of Complex Systems Program is a program of fundamental mathematics oriented research, the broad objectives of which are twofold. First, the program seeks to develop and analyze new, innovative, and robust modeling frameworks that may be adapted and generally applied across a variety of disciplines. The second goal is to develop both quantitative and qualitative models of specific complex phenomena in areas in which current models are either not fully based on first/basic principles or are based on empirical and ad hoc metrics for which the first/basic principles are not yet well known. Although they break down into more specific research directions, the three thrust areas of interest to the Modeling of Complex Systems Program are 1) development and analysis of new, general modeling frameworks, 2) geometric and topological modeling – which can be further broken down into more specific thrust areas, as noted below – and 3) small and large group social modeling and social informatics.

Metrics – in the general, non-mathematical sense of the word – are a natural part of the mathematical modeling framework. Traditional metrics, when they exist, often do not measure the characteristics in which observers in general and the Army in particular are interested. For many complex phenomena, new metrics need to be developed at the same time as new models. As is the case for the modeling effort, these metrics should preferably be in a complete mathematical analytical framework, which is to say, in part, that they should derive from the problem in question as opposed to a situation in which one forces the model to fit an *a priori* chosen metric. The research in modeling of complex phenomena supported by the Modeling of Complex Systems Program is primarily mathematical analysis and *not* numerical analysis or computational mathematics. One expects computation to play some role in any modeling endeavor, but the innovation in research carried out in the Modeling of Complex Systems program should be largely in the areas of modeling and analysis, and not in the computational techniques.

Furthermore, any modeling research effort that could be of benefit to military or intelligence applications but that might not fall directly under one or more of the program thrust areas will still be considered, particularly if the innovation in the modeling and analysis are significant and noteworthy.

The three major areas of research of the Modeling of Complex Systems Program are:

Modeling Frameworks and Analysis. Mathematical and physical modeling is fundamental to nearly every other direction of research in the physical, social, and computational sciences. A common element of modeling – even if the phenomenon in question is highly complex – is to incorporate simplifying assumptions that sacrifice realistic application and utility for computational ability. For Army and DoD applications, however, such simplifications often render the model impractical. Modeling frameworks are desired that are able to eschew the usual computational simplification assumptions and realistically capture, adequately govern and/or control, and effectively operate within the particular complexities of real world environments and phenomena, while still maintaining some degree of computational tractability. Of specific interest are causal and predictive modeling frameworks, hybrid model frameworks that capture both causal and predictive features, statistical modeling frameworks, and abstract categorical models (cf. Homotopy Type Theory).

Models of particular complex systems that address and are to be utilized for more specific purposes and objectives will be assessed within the context of one of the program's other modeling thrust areas described below. Research carried out under this section should address the general theory and analysis of mathematical modeling from a broader perspective.

Geometric and Topological Modeling. Representation of complex, irregular geometric objects and complicated, often high-dimensional, abstract phenomena, functions, and processes is fundamental for Army, DoD, and civilian needs. Such needs arise in the modeling of urban and natural terrain, geophysical features, biological objects (e.g. human brain mapping), information flow, and many other contexts. Any research that incorporates an innovative geometric and/or topological approach to address a problem with military, defense, and intelligence applications is welcome and will be considered, but there are two specific threads that are of particular interest to this thrust of the program: 1) geometric data analysis, and 2) multiscale geometric modeling, including dynamics and physical modeling on domains with fine, complex, geometric and/or topological structure.

Geometric data analysis includes – among other subfields – topological data analysis, subspace analysis, principal component analysis, and dimension reduction techniques. Current research directions of importance to Army applications include video, audio, and image processing (i.e. mathematical signal analysis), fast and accurate face/object recognition (i.e. reconstructing and matching geometric data through queries over a database), geometrically motivated methods and structures for working effectively with large – and often real-time extracted – data sets that may be corrupted in some way (e.g. missing or distorted data), and the application of persistent homology in the detection and classification of signals by shape. For instance, although good progress has been made in this direction, real-time capture, representation, and visual reproduction of 3D terrain – not just as a height field but with multivalent height functions and clearly defined topological obstructions – obtained directly from real-time or stored point-cloud data cannot be fully achieved with current techniques like the multitude of variations of piecewise planar surfaces that are presently studied. New approximation theory that does not require the classical assumptions – primarily smoothness – and that provides structure for the many new non-smooth approximation techniques currently under investigation is required.

Concurrently, research on the metrics by which we measure and evaluate the approximation is needed.

Additionally, approximation theory for information flow and other abstract phenomena in large wireless communication, sensor and social networks is also of interest. The approximation theory developed under support of this program is expected to provide building blocks for computational geometry, pattern recognition, automatic target recognition, visualization systems, information processing and network information flow.

Multiscale geometric modeling, analysis, and dynamics are of particular interest, both in the context of models of physical phenomena over real-world terrain and in the aforementioned complex, high-dimensional data structures. Models that make use of self-similar structures and recursively defined spaces (e.g. fractals, solenoids, etc.) would be of great interest in adapting or enhancing current techniques in areas such as data mining, fluid and heat flow, and search, evasion, deployment, and maneuver over complex terrain that exhibits self-similar properties (e.g. urban or mountainous terrain). Current techniques for dealing with complex dynamical processes and large, noisy, and possibly corrupted data sets could be greatly improved in both the time and efficiency realms by employing techniques from scale symmetry, which often allows one to reduce a large and unwieldy number of variables to a more manageable problem if the variables are appropriately scaled. Models that adapt self-similarity and automata theory, in particular, can oftentimes lead to mapping complex dynamical systems problems into an algebraic and/or topological category, which then may allow for entirely new tools and approaches to be used. Homotopy Type Theory and its applications are such an area that is of significant interest in military applications.

Small and Large Group Social Modeling. Both qualitative and quantitative analytical models of social group dynamics and information flow are required for operations, training, simulation (computer generated forces) and mission planning, as well as real-time analysis, processing, and dissemination of information. Current models have limited accuracy. Research focused on mathematically justified, practically useful, computationally tractable and data-tractable models is needed. ("Data-tractable" means "does not require more data or more detailed data than is realistically likely to be available."). Research on the metrics in which the accuracy of the models should be measured is also vitally important.

The broad term for this research pursuit would be social informatics, which is an important area in which more significant progress is needed, especially in the military and intelligence realms. Social informatics, briefly, is the study of the role played in society by information-based technology. This includes examinations of how the spread of information through technology effects social and organizational changes in society, as well as the converse – how social organization of information and use of technology to spread information are affected by social structures and practices. Modeling of the flow, dissemination, and possible evolution of belief systems and cultural factors through physical group migration or through social networking is an important tool in being able to predict where social and military issues might arise in the world.
This could lead to better preparation and the avoidance of "caught-off-guard" situations in global politics and military affairs.

Included within the social informatics realm are narrower but equally important research directions. These would include – but not be limited to – the dynamics of information flow across physical groups of people as well as social/technological networks, pattern detection in information flow and language, which would lead to more efficient surveillance and pre-emptive threat detection, as well as security in information transmission. In this latter direction, new and unique data structures and encryption techniques would be hugely beneficial. Complex but tractable multiscale data structures and viable fractal or self-similar encryption techniques – which heretofore have proved to be of academic but not very practical interest – are just a few examples of many that could prove useful.

Paralleling the pursuit of social informatics, information flow analysis, and pattern recognition in information and data is the quickly developing field of deep machine learning. The Army is particularly interested in developing programming models and training algorithms that can automate as much of these processes as possible. This involves a great deal of research into pattern recognition and data analysis, as well as model analysis. The interplay between causal, data-based models and predictive modeling are of special interest and an active area of military research.

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(2) Probability and Statistics

The research strategy of this program will focus on the following opportunities for crucial discoveries: innovative theories and techniques for modeling, analysis, and control of stochastic networks, stochastic infinite dimensional systems, and open quantum systems; innovative statistical theory and methods for network data analysis, spatial-temporal statistical inference, system reliability, and classification and regression analysis. Research in this area will provide the scientific foundation for revolutionary capabilities in counter-terrorism, weapon systems development, and network-centric warfare.

The program supports extramural basic research in stochastic analysis and control, and statistical analysis and methods in response to the Army's need for real-time decision making under uncertainty and for the test and evaluation of systems in development. Special emphasis is placed on methods for analyzing data obtained from phenomena modeled by such processes.

The two major areas of research are described below.

Stochastic Partial Differential Equations. Research on analytical and approximation methods for solving stochastic delay and stochastic partial differential equations and their related nonlinear filtering and control problems is one of the program objectives. The Hamilton-Jacobi-Bellman theory via dynamical programming principle and/or necessary optimality conditions in terms of maximum principles have to be further developed and refined for optimal control of these infinite dimensional equations. Modeling of rare event analysis of spatial-temporal random phenomenon requires a fundamental mathematical understanding of the theory of large deviations for infinite dimensional stochastic dynamical systems, in

particular stochastic partial differential equations driven by Brownian and/or Poisson space time noises.

Measure-Valued Stochastic Processes. An emerging and mathematically challenging area is the study of measure-valued process models of stochastic networks. One of the goals of this program is to develop general tools for the study of these processes, and their application to gain insight into the performance analysis, stability, control and design of this class of network models.

Weakly Interacting Stochastic Systems. Many physical and engineering systems can be modeled as a large collection of stochastically evolving agents or particles, whose dynamics are weakly coupled by an interaction that depends only on the empirical rise to many mathematically challenging questions. Among the many areas where progress is needed, the most important include the development of a general methodology to understand the long- time behavior of the solution to the limit measure-valued stochastic equation, and a related analysis into the implications of the long-time behavior of the limit for the stability or metastability of the stochastic N- particle system. Also of interest are issues of mean-field stochastic control, game theory, and in particular the design of stochastic controls via Lyapunov function techniques and the interplay between ergodicity and controllability in the stabilization of the stochastic system.

Quantum Stochastics and Quantum Control. With technological advances now allowing the possibility of continuous monitoring and rapid manipulations of system at quantum level, there is an increasing awareness of the applications and importance of quantum filtering and quantum control in engineering of quantum states, quantum error correction, quantum information, and quantum computation. To further understand the back action effects of measurements on quantum states and control of the system based on these measurements, novel mathematical development of non- commutative quantum stochastic calculus, quantum filtering and quantum control theory is necessary. Proposed mathematical research of this nature that has potential applications in quantum information and quantum computation is hereby solicited.

Statistical Testing and Validation of Network Models. The structure (network design), data sets and human element have a major impact on soldier performance. The need exists to develop new statistical techniques and theories to support the selection of optimal designs, validate predictive network models and modify data mining and inferential statistical techniques to use on ill-defined data and improve measurement. The research concentration areas include dynamical inference of structure in underlying models. In particular, ability to measure reaction of particular features buried in the network and not directly observable, and sequential analysis (changepoint detection) in networks.

Reliability and Survivability. To support future network-centric operations, the Army needs novel and efficient statistical tools for improving network reliability and survivability, and for analyzing data collected from sensor networks.

Bayesian and Non-parametric Statistics. Future emphasis in statistics on "predictive" models

vice explanatory models is important. Military operations call for predictive models based on a growing base of sensor-fueled data stores. Increased computational capability is also leading statistics in a new direction, away from using "classical" results which are really approximations to avoid computational issues. This suggests a need for increased emphasis on research in areas such as robust statistics, non- parametric statistics, non-linear models etc.

Statistical Analysis of Very Large and Very Small Data Sets. The state-of-the-art in statistical methods is well adapted to elicit information from medium-size data sets collected under reasonable conditions from moderately well-understood statistical distributions. However, Army analysts frequently have very large or very small data sets sampled from nonstandard, poorly understood distributions. Very often the data available does not measure the variable of interest and gives only indirect information. Thus the variable of interest is sampled in some ill-defined fashion. One needs to look at this problem in some generality and develop new theory to handle such problems with ill-defined data.

Geometric Methods for Statistical Inference. There is a research interest in unifying mathematical frameworks to capture the space of statistical models for inference and learning purposes. Models using differential geometric insights (such as Information Geometry) to characterize the manifold of probability density functions, to conceptualize measure-valued stochastic processes as paths on such manifold, and to understand the metric of model comparison and selection are welcome.

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(3) Biomathematics

The introduction of Biomathematics as a separate area of basic research recognizes the importance and specialized nature of quantitative methods, specifically mechanistic modeling, in the biological sciences. Biology involves a large number of entities that interact with each other and their environment in complex ways and at multiple scales.

This complexity makes biomathematics a highly interdisciplinary field that requires unique and highly specialized mathematical competencies to quantify structure in these relationships. In fact, progress in mathematical models of biological systems has traditionally been achieved by making convenient simplifications; major advances in Biomathematics research continue to require removing these assumptions (for example, stationarity, ergodicity and deterministic nature) and finding ways to effectively model the essential complexity. Modeling techniques currently utilized in the field range from agent-based approaches for determining the results of individual behavior, whether those individuals be molecules, zooplankton, or humans, to multi-compartmental modeling in physiology, epidemiology and neurobiology, to network models involved in understanding ecosystem and human social dynamics, as well as encompassing both deterministic and stochastic approaches. Research in control techniques is also valuable for its potential application in militarily important areas such as bio warfare and disease spread. Exciting new opportunities to advance the field are found in high risk attempts to develop modeling techniques in areas of mathematics, such as algebra and topology, not traditionally brought to bear on biological problems, advances in Bayesian statistics, a growing recognition

that the diffusion approximation is not necessarily adequate for many systems, and the availability of large amounts of complex biological data.

The ultimate goal of the Biomathematics Program focuses on adapting existing mathematics and creating new mathematical techniques to uncover fundamental relationships in biology, spanning different biological systems as well as multiple spatial and temporal scales. One area of special interest to the Program is Neuromathematics, the mechanistic mathematical modeling of neural processes. Recent advances in neuroscience provide important foundations to begin understanding how the brain works. Combined with experimental data, innovative mathematical modeling provides an unparalleled opportunity to gain a revolutionary new understanding of brain physiology, cognition (including sensory processing, attention, decision-making, etc.), and neurological disease. With this new understanding, improved soldier performance, as well as treatments for Post-Traumatic Stress Disorder, Traumatic Brain Injury, and other brain-related disorders suffered by the warfighter will be able to be achieved more effectively, efficiently, and ethically than via experimentation alone.

Thrust areas of the Biomathematics Program are as follows:

Fundamental Laws of Biology. The field of physics has long been "mathematized" so that fundamental principles such as Newton's Laws are not considered the application of mathematics to physics but physics itself. The field of biology is far behind physics in this respect; a similar process of mathematization is a basic and high-risk goal of the ARO Biomathematics Program. The identification and mathematical formulation of the fundamental principles of biological structure, function, and development applying across systems and scales will not only revolutionize the field of biology but will motivate the creation of new mathematics that will contribute in as-yet-unforeseen ways to biology and the field of mathematics itself.

Multiscale Modeling/Inverse Problems. Biological systems function through diversity, with large scale function emerging from the collective behavior of smaller scale heterogeneous elements. This "forward" problem includes creating mechanistic mathematical models at different biological scales and synchronizing their connections from one level of organization to another, as well as an important sub problem, how to represent the heterogeneity of individual elements and how much heterogeneity to include in the model. For example, the currently increasing ability to generate large volumes of molecular data provides a significant opportunity for biomathematical modelers to develop advanced analytical procedures to elucidate the fundamental principles by which genes, proteins, cells, etc., are integrated and function as systems through the use of innovative mathematical and statistical techniques. The task is complicated by the fact that data collection methods are noisy, many biological mechanisms are not well understood, and, somewhat ironically, large volumes of data tend to obscure meaningful relationships. However, traditionally "pure" mathematical fields such as differential geometry, algebra and topology, integration of Bayesian statistical methods with mathematical methods, and the new field of topological data analysis, among others, show promise in approaching these problems. Solutions to these types of multiscale problems will elucidate the connection, for example, of stem cells to tissue and organ development or of disease processes within the human body to the behavior of epidemics.

The "inverse" problem is just as important as the forward problem. From an understanding of the overall behavior of a system, is it possible to determine the nature of the individual elements? For example, from knowledge of cell signaling, can we go back and retrieve information about the cell? Although inverse problems have been studied for a long time, significant progress has been elusive. This thrust area involves innovations in spatial and/or temporal modeling of multi-level biological elements with the goal of achieving a deeper understanding of biological systems and eventually connecting top-down (data-driven) and bottom-up (model-based) approaches.

Modeling at Intermediate Timescales. Biological processes operate at a variety of timescales; understanding the dynamics of a system at intermediate timescales, as opposed to its long term, asymptotic behavior, is critically important in biology, more so than in many other fields. For example, an epidemic is a necessarily transient phenomenon. In addition, deterministic models are an approximation that often is not good enough to be informative about the system. Yet, intermediate timescales of nonlinear dynamics with stochasticity, both internal and external, are not well understood. This thrust area attempts to fill the gap in the basic understanding of modeling of systems, as well as their control, at intermediate timescales.

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(4) Computational Mathematics

The research strategy of this program is to focus on the following opportunities for crucial discoveries: innovative methodologies for solving currently intractable problems that take advantage of symmetry, conservation, and recurrence, that can adapt to both the evolving solution and to the evolving run-time resource allocation of modern computer architectures; novel algorithms that accommodate different mathematical models at different scales, interacting subsystems, and coupling between models and scales; methods that incorporate nonlocality through integral operators with advantageous representations. Research in this area will ultimately lead to the development of new mathematical principles that enable faster and higher fidelity computational methods, and new methods that will enable modeling of future problems.

Scientific computation is an essential component of scientific inquiry, complementing theory and experiment, and is also an essential element of engineering in both design and in failure autopsy. Simulations in support of inquiry, design, or autopsy often require expert knowledge in order to select methods that are compatible with the assumptions of the scenario at hand, require considerable skill to properly set up, require considerable time, memory, and storage on large scale parallel/distributed/heterogeneous systems to compute, and require considerable skill and effort to distill useful information from the massive data sets which result. Expert knowledge is also required to quantitatively estimate solution accuracy and to estimate the time and effort required to achieve a desired accuracy. Data has become ubiquitous and is potentially very valuable in increasing solution accuracy and/or decreasing the effort required to solve, but mathematically sound methods for incorporating data into accurate simulations are incomplete. Simulations are not always timely, with results often not being available until after

they are needed, for example in calculating failure of New Orleans levees during Katrina and in revising those estimates based on real time surge data. The emphasis in the Computational Mathematics program is on mathematical research directed towards developing capabilities in these and related areas.

For problems that are not time-limited, research areas of interest include but are not limited to the following:

Advances in Numerical Analysis. Novel methodologies are sought for solving currently intractable problems. New ways of taking advantage of symmetry, conservation, and recurrence are of interest, as are new ways of creating sparsity and new computational structures which can adapt to both the evolving solution and to the evolving run-time resource allocation of modern computer architectures. Rigorous analysis is sought for each in order to enable error bounds, error distribution, and error control.

Multiscale Methods. Problems of interest to the Army are increasingly characterized by the fact that behavior at microscopic scales has a large influence on performance of systems. To analyze these situations, algorithms are needed to deal with different mathematical models at different scales, interacting subsystems, and coupling between models and scales. The emphasis of this program is on mathematical methods which have some promise of wider application rather than methods limited only to specific application areas.

Fractional Order Methods. As an alternative to high order methods and other less-local operators, fractional operators are another nonlocal operator that have proven to work well in modeling and have the advantage of not enforcing dubious assumptions of smoothness, especially at discontinuities and interfaces. However, the nonlocality of fractional operators also typically introduces a significant increase in computational load. Advances in novel efficient computational methods for these operators are of interest.

Army systems often operate under rapidly-changing unpredictable and adverse conditions. It is desirable for models to be computationally simulated and fast enough to drive decision making, exercise control, and to help avoid disaster. Such simulations need to be created, run, and interpreted in better than real time. Research directed towards making this goal achievable is of interest, such as:

Reduced Order Models. Full scale simulations are often not realizable in real time. In order to investigate the behavior of systems under a variety of possible scenarios, many runs are required. Reduced order models are one way to enable this. Possible methods to create these models include adaptive simplification methods based on singular value decompositions and reduced order numerics. To be useful, all such models should be equipped with reliable estimates of accuracy.

Problem Solving Environments. To enable rapid decision making that is driven by simulation, it is necessary to set up simulations very quickly and obtain results in an understandable format. Matlab is one current tool for such a problem solving environment. What are other approaches?

Embedded Simulation. As algorithms become more efficient and computational devices shrink, it will become increasingly possible to use real-time simulation to drive control systems. New methods which address this goal are welcome, especially those which permit user- controlled and/or adaptively-controlled tradeoffs between speed and accuracy.

Decision Making. One valid criticism of numerical simulation is that it takes so long to set up, run, and post-process the results that they cannot be used in a timely manner to guide decision making. Mathematical ideas that help address this problem are of interest.

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iii. Network Science

The objective of the Network Sciences Division is to discover mathematical principles to describe ever present networks in all walks of life (e.g., organic, social, electronic) and, in particular, the emergent properties of networks. Study of Network Science is necessarily multi-disciplinary drawing on tools and techniques from statistical mechanics, information theory, computer science, control theory and social sciences to studies interactions at large scale, be they in swarms of insects or ant colonies, human societies, or networked autonomous systems. The basic principles discovered should, in turn, lead to creation of algorithms and autonomous systems that can be used to reason across data generated from disparate sources, including, sensor networks, wireless networks, and adversarial human networks. Research in this Division has applications to a wide variety of developmental efforts and contributes to the solution of technology-related problems throughout the Army's Future Force operational goals engendered by principles such as the Net-Centric Warfare and Third Offset strategy.

Research in the Network Science Division, while primarily driven by discovery of foundational principles, will, however, be cognizant of and contribute to providing crucial underpinning support to ARL's Network & Information Sciences Competency. In particular, the following goals within ARL's Network & Information Sciences Competency are explicitly addressed including: (i) assessment and control of behavior goal by creating new methods in design and controllability of composite and multi-genre networks; (ii) social effects and human-machine interaction through the exploration of social and cognitive networks, and generation of intelligent actions in a mix of information agents and humans; (iii) unconventional communication networks and adaptive by making information available at the tactical edge while taking limited bandwidth and human-information interaction modalities into account, and (iv) taming flash-flood of information available at the tactical edge.

The Network Science Division hosts four main programs in Wireless and Hybrid Communication Networks, Social and Cognitive Networks, Intelligent Information Networks, Multi-Agent Network Control, and an international research program in Network Science and Intelligent Systems. The boundary between these programs is fluid and, thus, a research topic might fall in more than one program area. Furthermore, there are shared interests between the Social Sciences program in Physical Sciences Directorate and Social and Cognitive Networks (SCN) program in Network Science, with SCN paying special attention to the human

dimension from a network science perspective, including study of connections between interdependent people (such as teams), between social systems and cognitive processing (such as collective learning and decision making), and between humans and machines, using tools and techniques from computer science to further the study of social and cognitive processes of humans embedded in large social, interconnected systems. It is perhaps worth emphasizing that research which elucidates and defines the common underpinning science cutting across different types of networks is particularly of interest to Network Science Division.

The Division's research areas are currently focused on five research areas that include one program focused on international research. The titles, scopes and points of contact for these programs, each of which address general aspects of basic research in network science, are listed in the following subsections. A small number of symposia, conferences and workshops are also supported in part or in whole to provide an exchange of ideas in areas of Army interest.

(1) Communications and Networks

This program is concerned with the investigation and advancing of network science applied to communication networks, in particular in wireless and tactical environments, with focus on Department of Defense and Army unique problems. These include, but not limited to, infrastructure-less wireless networks operating in congested and contested spectrum. Also of interest is the analysis of mutual interaction among the communications, social and information networks.

Wireless Network Theory. Research is required in the broad area of wireless network science including fundamental limits, performance characterization, novel architectures, and high fidelity simulation of multi-hop wireless networks with mobility, node loss, natural and man-made impairments and unpredictable, bursty traffic. Of particular importance is the extension of these findings in millimeter wave networks where spectrum is abundant, but connections are fragile and distances are short. Novel analytical tools and simulation techniques may be necessary to allow for the modeling of very large networking scenarios without losing the fidelity at the physical layer, which is critical in millimeter wave networks.

Emerging communications network paradigms of Software Defined Networking (SDN) and Network Function Virtualization (NFV) are also of interest as applied to wireless and hybrid networks. Concepts from SDN/NVF could be adapted for wireless ad hoc networks, using innovative methods. Complete centralization may not be desirable, but policy control and hierarchical control of semi-autonomous systems could be useful. Exploitation of SDN control architecture to tailor virtualized network resources according to the needs and objectives of the users is desired. Also, exposure of signaling traffic in wireless SDN creates significant security challenges which need to be resolved.

Mobile Ad Hoc and Sensor Networks. Networks serving Army needs operate in highly dynamic environments with limited or no infrastructure support. Available spectrum may be highly congested and contested, and mobile nodes may only have access to noisy local information with limited awareness of remote nodes in the network. Novel networking approaches may be needed to account for the lack of full network state information and

reduce the penalty incurred due to coordination while sustaining acceptable performance.

Adaptive and specialized machine learning techniques are needed for dynamic allocation of network resources based on operation needs, traffic characteristics, mobility, natural and man-made spectrum interference conditions, and security considerations. Techniques to discover and capitalize on communication and networking opportunities. Networking and sensing architectures for cognitive mobile ad hoc networks needs to be developed with qualitative and quantitative performance measures, and the impacts of mobility, fading, and multi-user interference needs to be investigated. Concepts and constructs observed in networks encountered in nature could inspire adaptation strategies for ad hoc wireless networks.

Networking in combat operations may need to cope with the presence adversarial actions of various types, including strategically inserted spectral impediments. New signal processing, information theory, game theory and network science methodologies are needed to provide reliable and efficient communications in the presence of various adversarial actions. The analysis and characterization of fundamental tradeoffs among conflicting objectives such as Low Probability of Detection (LPD) vs. rate of communications vs. operating in a limited frequency spectrum are needed, along with novel techniques to achieve optimally located areas in the trade-off boundaries.

Providing energy efficient sensor networking under possibly hostile operating conditions presents considerable challenges. Such networks involve short packets and very large number of users, for which standard network access methods are known to be neither spectrum, nor energy efficient. Investigation of fundamental limits in network access methods which pertain to short packets, many users and hostile environments is desired, along with the discovery of protocols which could approximate these bounds.

Novel and Revolutionary Methods in Networking. The synergy among social networking and communication networking, particularly in a tactical mobile ad-hoc scenario, is a research area that could advance the design of new communication approaches. There are many social networking aspects that are common to mobile ad-hoc networking needs such as distributed decision making, robustness, cooperation, self-organization, cluster formation, search and exploration, to name a few. Social Networking Analysis concepts have been recently used in routing and storing of information for tactical wireless networks, with some encouraging results.

Distributed authentication methods, such as block-chain could be useful in tactical environments, but they may require excessive computation and storage burden. Rethinking of distributed authentication methods to fit tactical environments where links may be unreliable, energy and storage is limited is desired.

Among novel and revolutionary methods in networking, exploration of quantum information processing, teleportation and networked quantum information theory is of interest.

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(2) Social and Cognitive Networks

The goal of the Social and Cognitive Networks program is to understand human behaviors and cognitive processes leading to collective level phenomena particularly relevant in military settings with an emphasis on high performance teams and computational social science. Social networks are the underlying structure of interaction and exchanges between humans within both strategically designed and emergent or self-organized systems. Social networks allow for collective actions in which groups of people can communicate, collaborate, organize, mobilize, attack, and defend. The changing nature of DoD's missions greatly increase the need for models that capture the cognitive, organizational, and cultural factors that drive activities of co-present, virtual, or distributed groups, teams, and populations. Better understanding the human dimension of complexity will provide critical insights about emerging phenomena, social diffusion and propagation, thresholds, and tipping points.

The Social and Cognitive Networks program supports projects that contribute substantive knowledge to theories about human behavior and interaction and make methodological advancements in modeling and analyzing social network structures. The U.S. Army is particularly interested in research that uses defense-relevant empirical data to feed into computational and mathematical models of human interaction. As such, this program funds projects successful in blending theories and methods from the social sciences with rigorous computational methods from computer science and mathematical modeling. Advances in this program are expected to lead to development of measures, theories, and models that capture behavioral and cognitive processes leading to emergent phenomena in teams, organizations, and populations.

Human Behavior and Interaction. This program supports research from disciplines such as communication, health and behavioral science, I/O and social psychology, library and information science, management science, and sociology that use a social networks lens to focus on the ways people think and interact whereby creating higher-order systems. Topics of interest include social influence, leadership, trust, team science, cooperation and competition, and crisis management. Such social influence and opinion dynamics research could focus on the formation and dissolution of civic-minded and violent ideological networks, mobilization of benign to hostile political movements, propagation of and enduring changes in attitudes leading to populations reaching consensus or contested states, and network-based interventions. Furthermore, topics of particular interest include social effects of human-machine teaming; multi-team systems and multilevel (nested) systems; and health topics related to education, healthcare behaviors, disease propagation, and wellness from a social networks perspective.
Information and Knowledge Management. This program supports social network centric research to study the ways people learn individually and collectively and how they utilize that information for decision making and goal attainment. Examples of relevant topics include transactive memories, public goods, collective action, information sharing, information fidelity, diffusion and propagation dynamics, and collective decision-making. Diffusion dynamics research will develop mechanistic understanding of opinion and behavior change associated with influence, contagion, and other social propagation

processes. Collective decision-making research will contribute fundamental theories and models to predict, evaluate and simulate how teams organize, exchange information, build knowledge, influence, adapt, learn, and build consensus using cooperative strategies and emergent capabilities.

Social Network Analysis. In addition to the topical areas identified above, this program supports methodological advancements for social network analysis. Methodological research in this program will focus on important advances in exponential random graph models (ERGMs or p^*), object oriented agent-based models, computational models, and dynamic simulations that resolve network modeling issues. Such research will focus on scalability of networks, hierarchical or multilevel (nested) systems, longitudinal networks, social influence models, network resilience, techniques to deal with missing, incomplete, or inaccurate network data, and techniques to deal with visualizing multilevel multimodal networks. Scalability and dimensionality research will identify overarching mechanisms that span scales and dimensions of human systems that will parameterize, model, and predict both small group and big data network models. Data accuracy research focuses on investigating effects of measurement error on metrics and inferences due to incomplete (missing or inaccurate) network data. These projects could include research examining small group dynamics within big data sets; multi-level models that account for nested cognitive, social, cultural, physical dimensions of systems; or link and subgroup estimation algorithms to deal with incomplete data and clandestine activities.

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(3) Intelligent Information Networks

The overall objective of the Intelligent Information Networks program is to augment human decision makers (both commanders and soldiers) with enhanced-embedded battlefield intelligence that will provide them with the necessary situational awareness, reconnaissance, and decision making tools to decisively defeat any future adversarial threats which is in line with the DoD's adoption of net-centric warfare, variously defined as flattening the information space to interconnect soldiers and commanders to provide instantaneous access to information, knowledge, and situational awareness. Given this goal, it becomes necessary to understand (a) fundamentals of what intelligence means in the context of autonomous systems and how to build intelligent systems especially as it relates to interaction amongst a network of humans and machines, and (b) foundational algorithmic issues in representation and reasoning about networks inherent in societies and nature.

Integrated Intelligence, Theory of Mind, and Collective Intelligence. Intelligence emanates from several components acting in synergistic ways, be it human cognition that embodies cumulative effects of various separate components of the human brain or the collective intelligence of a network of agents (humans, birds, insects, etc.). Fundamental questions that need to be answered include: What is the least amount of knowledge necessary to boot-strap learning in autonomous systems (or in a network)? How can joint reasoning over various components be carried out (vision, knowledge representation, reasoning, planning,

for instance) to obtain a sum that is more than its parts? Are there viable, computable theories of mind that can realistically implement reflection and meta-cognition? Can wisdom of crowds be harnessed to solve problems of importance to societies and problems that are deemed computationally hard? In particular, can a man in the middle of a man-machine ensemble, or, more appropriately, can a crowd and machine ensemble solve inherently hard problems? What exactly are the limitations of wisdom of crowd, when the crowd is made of non-experts? Is there are a way for problems to be broken up so that a team of humans and machines can solve them together? Are there approaches to mechanism design that teases out intelligence inherent in a crowd (or society) of interest in this thrust? These are some of the questions whose solution would likely address basic research problems that are of interest to the program.

Information Networks. In order to model network effects it is necessary to algorithmically represent large networks and reason about them. Unfortunately, information about networks is seldom complete – data available might be missing crucial pieces of information, might have contradictory pieces of information, or could be approximate (with associated notions of uncertainty). Representing and reasoning about these networks requires advances in knowledge representation, graph and data mining, natural language processing, algorithmic graph theory, machine learning, and uncertainty quantification and reasoning. Examples include the emerging area of Graphons which provide new tools for generating and reasoning about graphs that occur in practice (satisfying power law distributions), but also provide new tools for Machine Learning. In particular, a major goal of this thrust are tools and techniques that allow data driven approaches to capturing latent relationships with powers to both explain and predict. Advances in this thrust would not only lead to improved autonomous systems and algorithms, but also enhanced-embedded battlefield intelligence with tools for creating necessary situational awareness, reconnaissance, and decision making. Finally, it should be noted that algorithmic notions of approximations, tight performance bounds, probabilistic guarantees, etc., would be major concerns of the solution space. Large graphs and voluminous data characterize problems in Network Science.

Adversarial Reasoning. Development of appropriate mathematical tools to model and reason about societies and cultures, that brings together tools from Game Theory, Social Sciences and Knowledge Representation. Research of interest includes, but is not limited to, Game Theory for security applications while accounting for bounded rationality, development of Game Theory based on data regarding cultural and adversarial groups, and Behavioral Game Theory that can explain intelligence in groups and societies.

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(4) Multi-Agent Network Control

The objective of the Multi-Agent Network Control program is to establish the physical, mathematical and information processing foundations for the control of complex networks. The research program is concerned with developing novel mathematical abstractions and methods for the modeling and control of both individual agents as well as the collective

behavior of large scale networks of heterogeneous multi-agent systems. In this regard, the term "agent" can span the biological, physical, and information and communication domain. Autonomy is central to program efforts as anticipated dynamics of the future battle space will require a greatly increased level of autonomy to enable the necessary mobility, sensor coverage, information flow, and responsiveness to support the military goals of information superiority, dominant maneuver, and precision engagement.

Distributed Control for Complex Networks. Distributed control techniques have played a major role in the study of networked systems. For example, they have been successfully used in robotics for replicating self-organized behaviors found in nature (e.g. bird flocking, fish schooling, and synchronization) and in developing applications such as formation control, rendezvous, robot coordination, and distributed estimation. A fundamental concept underlying these techniques is the notion of consensus. However, many control problems in complex networks cannot be framed as consensus problems. Hence, there is need for developing a new generation of distributed control methods for achieving more sophisticated control goals that are not amenable to a consensus-based formulation. In large-scale networks of interdependent dynamical systems this is likely to require hybrid control architectures that combine top-down and bottom-up design methods formally grounded in graph theory, dynamical systems theory, game theory, computational homology, and topology, amongst other disciplines. Research in this area should contribute to a better understanding of the tradeoffs between what can be achieved by a multi-agent system (e.g. controllability) versus (i) information processing requirements, network topology and computational overhead (ii) individual-agent control actuation capabilities, and (ii) degrees of autonomy and cognitive-behavioral issues arising from human-system interaction.

Analysis of Complex Co-Evolving Networks. The high-dimensionality and complex, evolving topologies in complex networks of heterogeneous agents with possibly asymmetric interactions requires new mathematical techniques for characterizing out-of-equilibrium dynamics and the likely equilibrium outcomes that may emerge over different time spans. Due to random perturbations, transitions between equilibria are inevitable with some transitions occurring more readily than others. Thus for a complete understanding of the dynamics of interacting agents, one must understand how and when equilibrium is likely to unravel, and which new equilibrium, if any, is likely to arise in its place.

Information Structure, Causality, and Dynamics for Control. Understanding information processing within and for controlling complex networks requires new tools for causality and topological inference. Major programmatic interests center on formulating abstractions of cognitive processes and perception for fundamentally changing the way information is exploited to enable control and re-shaping the actions of multiple agents and complex networks. Further questions include: How does control as an objective effect communication and information processing in complex networks? What are the fundamental limits of causality? How do we infer causality and perform estimation in complex networks.

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(5) Network Science and Intelligent Systems (International Program)

As one of the ARO International Programs, the Network Science and Intelligent Systems Program is focused on supporting research at universities outside of the U.S., with the goal of providing key connections with world-class researchers outside the U.S. and supporting the most forward looking and promising research in network science.

Refer to Section II.A.2 of this BAA for a detailed description of this international research program's research goals, including the titles, scopes and points of contact for these programs.

2. INTERNATIONAL RESEARCH INTERESTS

The U.S. Army Research Office has international research programs which are focused in specific research areas supporting the 10 scientific divisions. These research areas and information provided in the following are opportunities for foreign organizations and foreign public entities.

a. Energy Transport and Storage

As one of the ARO International Programs and part of the ARO Chemical Sciences Division portfolio, the Energy Transport and Storage Program is focused on supporting research at universities outside of the U.S., with the goal of building international partnerships and laying the foundational work upon which energy storage and power generation technologies depend. Potential investigators should contact the Program's TPOC for any questions regarding the geographic regions that can be considered for research proposals in this area.

This program targets insightful and high-risk, fundamental research which addresses the core underlying limitations of energy transport/storage. Central to the mission of this program is the exploration of how materials and cell design can be tailored to enable targeted electrochemical reactions—while eliminating side reactions, hazards and other impediments, thereby surmounting hurdles and exploiting opportunities in chemical energy storage.

Energy Transport. This thrust supports research aimed at evaluation protocols for energy-relevant materials and the scrutiny of new solid ion conductors and liquid/slurry active materials. There is a tendency to focus upon the most favorable aspects of energy-relevant chemistries and materials, but such reports often either fail to identify or neglect the key limiting characteristics which researchers in general and the Army in particular require to overcome the constraints which restrict breakthroughs in a given energy technology. Projects which actively seek to obtain a global understanding of the underlying principles regarding how chemicals/materials impact the stability and performance of energy storage technologies are of Army interest. Advances in solid electrolytes hold the promise of revolutionizing energy storage technologies, but numerous factors such as limited ionic conductivity, poor ion selectivity, high reactivity, composition changes during processing or difficult processing

methods, high contact resistance, unfavorable mechanical properties, defect propagation during cycling due to mechanical deformation, cost barriers, etc. remain major obstructions to the integration of solid electrolytes/separators into devices. Innovative approaches to propel these critical cell components forward are sought. The identification of promising, new liquid (or slurry) active materials (i.e., anolytes or catholytes) may potentially enable new cell designs which greatly simplify battery production, scalability and the tunable modularity of cells, thus enabling their assimilation into diverse Army-relevant energy storage applications. Other innovative project themes are also welcome.

Thermal Energy Storage. This thrust's focus is on thermal energy storage phase change materials (PCMs). PCMs permit both passive and active heating/cooling that can significantly reduce or eliminate the necessity of conventional heating and cooling methods (for buildings, refrigeration, electronics, etc.). Many PCM applications, however, are restricted due to their high cost, low thermal conductivity, change in density, limited stability of thermal properties and tendency to subcool. The discovery and characterization of new PCMs (e.g., based upon solvates, eutectics, etc.) may overcome these challenges thereby enabling a path forward for their widespread implementation.

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b. Synthetic Biology

As one of the ARO International Programs and part of the ARO Life Sciences Division portfolio, the Synthetic Biology Program is focused on supporting research at universities outside of the U.S., building international partnerships and laying the foundational work on which applications of synthetic biology will depend. Emphasis is on using synthetic biology techniques to understand basic biology and to design biological systems and processes with high reliability, scalability, and predictability. Potential investigators should contact the Program's TPOC for any questions regarding the geographic regions that can be considered for research proposals in this area.

A major program thrust is investigation of the ways in which biological systems use and control evolutionary processes to become robust, complex, and adaptive. Investigations of interest include mutational hot spots, genetic rearrangement, horizontal gene flow, hyper stable DNA regions, recurrent editing, and maintenance through generations of "unused" adaptations, for example adaptations that allow resistance to dehydration maintained for generations in the absence of selective pressure. These naturally occurring processes may be combined with techniques that do not occur in nature, such as gene shuffling and directed editing, to create organisms that are both engineered and adapted. Combined with a systems biology approach, principles of encoding complexity and adaptivity can be derived. Sophisticated selective techniques are also sought, to drive evolutionary processes to desired ends and to create organisms with desired characteristics.

A second research thrust is the development of robust, predictable systems. Emphasis is not on what such a system does so much as how it can be created, maintained, and activated, to

include consideration of the time course of reactions, energetics, methods of preservation and storage, methods of activation, stability, and reliability.

The third thrust of the program is on the creation and maintenance of hybrid prokaryotic-eukaryotic symbiotic systems. Such systems can potentially combine the relative ease of engineering of prokaryotes with the robustness and processing capability of eukaryotes. Areas of interest include the reliable formation of stable intracellular prokaryotic forms, release and reformation of extracellular prokaryotic forms, transport of prokaryotic products into eukaryotic cytoplasm, membranes, and extracellular space, and eukaryotic processing of prokaryotic products. Studies of the innate immune system of both plants and animals are also of interest, as well as intracellular immune processes.

TPOC: Dr. Valerie Martindale, valerie.e.martindale.civ@mail.mil, +81-46-407-9309 (Tokyo, Japan)

c. Human Dimension

As one of the ARO International Programs and part of the ARO Life Sciences Division portfolio, the Human Dimension Program is focused on supporting multidisciplinary research at institutions outside of the U.S., with the goal of identifying and modeling the co-evolutionary multiscale dynamics of human neural, cognitive, physical and social systems. Potential investigators should contact the Program's TPOC for any questions regarding the geographic regions that can be considered for research proposals in this area.

The Human Dimension Program supports multidisciplinary basic research in areas that include neural and cognitive sciences, behavioral and social sciences and human factors and neural engineering with an emphasis on modeling, predicting and enhancing human perceptual, cognitive, affective, physical, and social performance in individuals, groups and societies. An overarching goal of the program is to provide foundational knowledge of neural, biophysiological and cognitive-based mechanisms underlying individual, group and societal cognition and performance across multiple time scales. In the long term, research in this area may enable new training tools to predict and optimize cognitive/physical performance and team intelligence, interfaces enabling humans to more efficiently control machines and psychophysiologically-based predictive models of complex individual – societal dynamics. Basic research opportunities are sought in two primary research thrusts within this program: (i) Cognitive-Physical Interactions and (ii) Cognitive-Social Interactions.

Cognitive-Physical Interactions. The Cognitive-Physical Interactions thrust seeks to support high-risk seed projects that use multimodal approaches to uncover dynamic and multiscale interactions of neural-cognitive and physiological systems. The goal of this thrust area is to advance the experimental and analytical tools available to develop comprehensive understanding of the impact of group and individual state-trait variability on human performance, human-systems interfaces and team intelligence. Research topics are supported in diverse areas that can include the neurobiological mechanisms of expert skill learning, closed-loop brain-computer interfaces and novel mind-body interfaces such as the microbiome-gut-brain axis.

Cognitive-Social Interactions. The Cognitive-Social Interactions thrust seeks to develop new theories to understand the dynamic interrelationships between individual/group cognition, decision-making and the role that these influences play on interactions with large and small social systems. Multidisciplinary seed projects are supported that seek to advance the necessary analytical and experimental tools required to describe the underlying mechanistic interactions as they co-evolve in time and space. Research topics are supported in diverse areas that may include modeling the impact of mindfulness on state transitions of human cognitive, physical and social systems and describing the longitudinal neural, cognitive and social mechanisms mediating development of leadership, expertise and intelligent teams.

TPOC: Dr. Frederick Gregory, frederick.d.gregory5.civ@mail.mil, +44 (0)1895-626517 (London, UK)

d. Quantum Scale Materials

As one of the ARO International Programs and part of the ARO Physics Division portfolio, the Quantum Scale Materials Program is focused on supporting multidisciplinary research at institutions outside of the U.S., with the goal to accelerate new discoveries in quantum scale materials. Potential investigators should contact the Program's TPOC for any questions regarding the geographic regions that can be considered for research proposals in this area.

Specific research topics of interest include, but are not limited to: topological states of matter and photons, matter and photons that can support anyon quasiparticles, quantum phase transitions, non-equilibrium quantum dynamics, novel materials for quantum information processing, quantum metrology with atoms, ions and photons, quantum networks, and novel quantum information effects, such as effect of free will (measurement independence) on quantum algorithms, such as teleportation, quantum communication and quantum computing.

Additionally, over time new areas of research in fundamental physics surface that provide previously unforeseen opportunities for accelerating scientific progress, and this BAA is intended to cover these cases.

TPOC: Dr. Thomas B. Bahder, thomas.b.bahder.civ@mail.mil, +81-46-407-9308 (Tokyo, Japan); (984) 209-0096 (U.S. cell)

e. Innovations in Materials

As one of the ARO International Programs and part of the ARO Materials Science Division, the Innovations in Materials Program is focused on supporting multidisciplinary research at institutions outside of the U.S., with the goal of accelerating new discoveries in materials science. Potential investigators should contact the Program's TPOC for any questions regarding the geographic regions that can be considered for research proposals in this area.

The Innovations in Materials program seeks to determine unique strategies and designs for

optimizing materials with uncharacteristic or unexpected properties, architectures, and compositions. Research is focused on, but not limited to, areas such as: reconfigurable materials, predictive design of materials, multi-component materials incorporating hierarchical constructs, materials compositions and architectures for unprecedented property development, functional integration of materials, analytical techniques for interrogating multi-dimensional evolution of structures, properties and failure, and defect science and engineering.

Over time, new areas of research in fundamental materials science can develop that provide previously unforeseen opportunities for accelerating scientific progress, and this BAA is intended to cover these cases as well.

TPOC: Dr. Pani Varanasi, chakrapani.v.varanasi.civ@mail.mil, (919) 549-4325

f. Network Science and Intelligent Systems

As one of the ARO International Programs and part of the ARO Network Science Division portfolio, the Network Science and Intelligent Systems program is focused on supporting multidisciplinary research at institutions outside of the U.S., with the goal to accelerate new discoveries in network science and intelligent systems. Potential investigators should contact the Program's TPOC for any questions regarding the geographic regions that can be considered for research proposals in this area.

Wireless Communications and Information Networks. Networks serving Army needs must operate in highly dynamic environments with limited infrastructure support. Networks will be disconnected, intermittent, and limited (DIL) environment, with limited state information and dynamic network connectivity and intermittent link connectivity as well as dynamic traffic load with various QoS constraints and priorities. Metrics, fundamental limits, and performance need to be characterized for tactical networks as well as new theory that will lead to reliable and efficient communications that meets QoS constraints. New algorithms and protocols that are more robust in the presence of various adversarial attacks are required.

One specific area of interest is SDN that can operate within tactical DIL networks. Standard SDN are centralized utilizing a reliable control plane, which are not available in this environment. Research is needed to investigate if SDN can be used in this environment and how architectures and control algorithms need to be modified to meet QoS requirements.

Social Network Analysis and Visualization. Mathematical models for dynamics of large social networks are of interest. Modeling of dynamics of the social network are of interest to include both (and possibly co-evolving) structure and content (e.g., opinion dynamics). Hierarchical, multi-level, and composite network models are of interest to model interactions between networks. Scalability issues should be investigated to understand when they are applicable and models should be vetted against established sociological concepts and, if possible, using experimental data. Multi-scale visualization of social network data is important for presenting results of analysis to users and assisting in manual analysis. Missing, incomplete, and inaccurate data are issues that should be considered in network analysis techniques.

Dynamics of Interdependent and Multilayer Networks. In the emerging field of networks science, the importance of research into interdependent and multilayer networks, such as communications, social, and infrastructure networks, is becoming evident. The mathematics to understanding how to model, predict, and control such multi-layer and interdependent networks is an important research area.

Intelligent Systems. This part of the BAA invites proposals in the area of Network Inference, Data Mining, and Algorithmic Game Theory that supports aspects of Network Science, including understanding large groups, especially adversarial non-state actors. Work that advances Network Science by bringing new techniques from Game Theory, Machine Learning, Graph Algorithms, Reasoning under uncertainty, are welcome.

TPOC: Dr. Derya Cansever, derya.h.cansever.civ@mail.mil, (919) 549-4330

3. ARO SPECIAL PROGRAMS

a. Short-Term Innovative Research (STIR) Program

The objectives of the STIR program are to support rapid, short-term investigations to assess the merit of innovative new concepts in basic research. STIR program awards provide an excellent opportunity to showcase new concepts and explore new areas in basic research. Historically STIR program awards have helped shape new directions in research for the Army.

i. Eligibility. Proposals are sought from institutions of higher education, nonprofit organizations, state and local governments, foreign organizations, foreign public entities, and for-profit organizations (i.e. large and small businesses). Prospective applicants of a STIR proposal are encouraged to contact the appropriate TPOC/ Program Manager identified earlier in the research areas of this BAA, to ascertain the extent of interest in the specific research project.

ii. Research Sought. Proposals in the amount of $60,000 or less are sought for research in the areas identified earlier in the research areas of this BAA.

iii. Proposal Preparation.

(1) Eligible applicants should submit proposals that are no more than twenty (20) pages in length, inclusive of the budget, transmittal letter, and attachments. No brochures or explanatory material should be submitted with the proposal.

(2) Proposed research efforts must be "stand alone" and not predicated on the use of any facilities other than those under the direct control of the applicant. Research must be completed within nine (9) months of award of the agreement.

(3) The research proposal should follow the format set forth in Section II.D (Application and Submission Information) of this BAA. Limited rights in technical data and restricted rights in computer software should be identified as an attachment to the proposal. Otherwise, it will be

concluded that the proposal does not contain any such limitations or restrictions

(4) No capital equipment may be purchased under a STIR Program award. Travel costs must not exceed $500. Report preparation costs must not exceed $100. Fee is not permitted under STIR Program awards. Due to the relatively small dollar amount and short-term nature of these awards, applicants are encouraged to maximize the benefit derived from this funding by prioritizing labor and employing other cost-saving measures in support of the STIR program effort. In particular, applicants are strongly encouraged to contribute as a cost-share or significantly reduce the indirect costs associated with proposed efforts.

(5) The principal investigator(s) (PI) should disclose and explain the relevance of the proposal to the research interests identified earlier in the research areas of this BAA.

(6) A brief, final technical report is required. Please note that your award document will reference Form 18, "Reporting Instructions," as found at http://www.arl.army.mil/www/default.cfm?page=29. You shall use these reporting instructions for format instructions only; the due date for receipt of a final technical report is thirty (30) days from completion of the award.

b. Young Investigator Program (YIP)

YIP awards are one of the most prestigious honors bestowed by the Army on outstanding scientists beginning their independent careers. The objective of the YIP is to attract outstanding young university faculty members to pursue fundamental research in areas relevant to the Army, to support their research in these areas, and to encourage their teaching and research careers. Young investigators meeting eligibility requirements may submit a YIP proposal. Outstanding YIP projects may be considered for a Presidential Early Career Award for Scientists and Engineers (PECASE). For FY20 only, this program will be supplemented by additional funding provided by the Defense Established Program to Stimulate Competitive Research (DEPSCoR). Three additional awards may be made to principal investigators in DEPSCoR-eligible states as defined in 10 U.S.C. 2358, as amended by Pub. L. 115-91, div A, title II, sec. 219. Potential awards will be limited to Institution of Higher Education (IHE) in States/Territories that are eligible under the DEPSCoR program authority. Tenured or tenure-track faculty members with appointments at IHE, in the following States/Territories, are eligible to apply for DEPSCoR opportunities: Alabama, Alaska, Arizona, Arkansas, Connecticut, Delaware, District of Columbia, Guam, Hawaii, Idaho, Indiana, Iowa, Kansas, Kentucky, Louisiana, Maine, Minnesota, Mississippi, Missouri, Montana, Nebraska, Nevada, New Hampshire, New Mexico, North Dakota, Oklahoma, Oregon, Puerto Rico, Rhode Island, South Carolina, South Dakota, Tennessee, U.S. Virgin Islands, Vermont, West Virginia, Wisconsin, and Wyoming.

i. Eligibility. This program is open to U.S. citizens, U.S. Nationals, and Permanent Resident Aliens holding tenure-track positions at U.S. institutions of higher education, who have held their graduate degrees (Ph.D. or equivalent) for fewer than five years at the time of application. Faculty at an institution of higher education which does not designate any faculty appointments as "tenure track" are eligible if that fact is so indicated in the proposal, and the

supporting letter from the institute states that the faculty member submitting the proposal will be considered for a permanent appointment.

ii. Research Sought. Proposals are encouraged for research in areas described earlier in the research areas of this BAA. Proposals may be submitted at any time. As is the case for all other research programs, discussions with the cognizant TPOC/ Program Manager identified earlier in the research areas of this BAA is strongly recommended before submission of a formal proposal. An award in each topic area is not guaranteed. YIP awards will not exceed $120,000 per year for three years.

iii. Proposal Preparation.

(1) An individual applying for a YIP award must submit a proposal and a supporting letter, both through official channels in the institution of higher education where the individual is employed. Any resulting award will be made to the institution, not to the investigator. The proposal should follow the format set forth in Section II.D (Application and Submission Information) of this BAA.

TPOC: Contact the relevant Program Manager identified earlier in the research areas of this BAA.

(2) The supporting letter must be from the individual's Department Chairperson, Dean, or other official who speaks for the institution of higher education, and should address support for, and commitment to, the applicant. Strong university support for the applicant is essential. This support can include the applicant's nine-month academic salary, release time from administrative responsibilities, the purchase of equipment, support for the applicant's graduate students, waiver of indirect costs, departmental cost sharing, start-up funding, and so on. It must be clear that the institution of higher education views the individual as a truly outstanding, faculty member, and is making a long-term commitment to the proposal and the research.

iv. Evaluation Criteria. The evaluation criteria to be used in determining which proposals are selected for funding are described in Section II.E.1.a and Section II.E.1.b of this BAA. YIP proposals will be selected for award on a competitive basis after a peer scientific review.

v. Continued Support. Support under the YIP is limited to three years. Upon completion of the YIP award, a young investigator, through their institution, may apply and be considered for continued support in the research areas of this BAA.

c. Presidential Early Career Award for Scientists and Engineers (PECASE)

i. An individual may not directly apply for a PECASE award. Instead, once a year, ARO technical program managers will nominate PECASE candidates from among all ARO YIP and other proposals and whitepapers (if any) received. A technical program manager will make the PECASE nomination based on strong endorsement of the proposal by the external scientific

reviewers and on the potential shown by the individual to contribute to science and to the mission of the Army.

ii. Following nomination of a PECASE candidate, a supplemental PECASE proposal will be requested in which the candidate will indicate how PECASE funding would augment the YIP award. PECASE awards are not to exceed $200,000 per year for five years. The following supporting information at minimum is required in the PECASE proposal:

(1) Letters (non-federal government) of recommendation;
(2) Detailed scientific biographical information including a description of the candidate's leadership in the scientific community;
(3) Description of the proposed candidate's publications (such as refereed journals, peer-reviewed conference papers, and books or book chapters; however, this is not an inclusive list);
(4) Description of the candidate's presentations (such as invited talks and plenary presentations; however, this is not an inclusive list);
(5) Summary of the candidate's past research accomplishments;
(6) Summary of the candidate's community outreach efforts; and
(7) Letters of commitment from institution(s) of higher education.

iii. Complete PECASE proposal packages will be evaluated by scientific reviewers. The proposals which demonstrate the greatest potential to contribute to science and to the mission of the Army will be rank ordered by an Army PECASE Evaluation Committee. The evaluation criteria to be used in determining which proposals are selected for funding are described in Section II.E.1.d of this BAA.

iv. Continued Support. Support under PECASE is limited to five years from date of award. Upon completion of the PECASE award, an individual, through their institution of higher education, may apply and be considered for continued support in the areas identified earlier in the research areas of this BAA.

TPOC: Contact the relevant Program Manager identified earlier in the research areas of this BAA.

d. Research Instrumentation (RI) Program

RI is designed to improve the capabilities of U.S. institutions of higher education to conduct research and educate scientists and engineers in areas important to national defense. Of the funds available to support ARO mission research described in this BAA, funds may be provided to purchase instrumentation in support of this research or in the development of new research capabilities.

i. Eligibility and Areas of Interest. It is highly recommended that potential applicants contact the appropriate TPOC/ Program Manager identified earlier in the research areas of this BAA for advice and assistance before preparation of an instrumentation proposal.

ii. Content of Request for Instrumentation. The request for instrumentation shall include:

(1) A concise abstract (approximately 300 words but not to exceed 4,000 characters) that describes the instrumentation requested and the research to be supported by that instrumentation.

(2) A budget that addresses the instrumentation to be purchased, cost per item, and total cost. Indicate the proposed source of the instrumentation and the name and telephone number of a contact at that source. The budget should indicate the amount of funds to be contributed by other sources toward the purchase of the instrumentation.

(3) A description of how the proposed instrumentation will: (i) establish new research capabilities, (ii) contribute to research currently proposed to DoD, or (iii) enhance the quality of research currently being funded by ARO.

(4) A description of how the proposed instrumentation will interface with or upgrade other research facilities and instrumentation now available.

(5) A description of the amounts and sources of ongoing or proposed support for the research to be supported by the instrumentation.

Note: Costs associated with equipment/facility modifications are generally considered unallowable and require the review and approval of the Grants Officer.

iii. The evaluation criteria to be used in determining which proposals are selected for funding are described in Section II.E.1.a and II.E.1.c of this BAA.

e. Conference and Symposia Grants

i. Introduction. The Army supports conferences and symposia (as defined in the DoD Travel Regulations) in areas of science that bring experts together to discuss recent research or educational findings or to expose other researchers or advanced graduate students to new research and educational techniques. The Army encourages the convening in the United States of major international conferences, symposia, and assemblies of international alliances.

ii. Eligibility. Notwithstanding the Army's authority to provide grant support for such events, only non-commercial scientific, technical, or professional organizations that qualify for tax exemption may receive a conference grant/symposia grant. Those who meet this requirement should also be aware that the DoD does not permit "co-sponsorship" (as defined in DoD 5500.07-R) absent additional high level staffing and approval. In other words, the conference grant support identified in this BAA is NOT DoD sponsorship or co-sponsorship since ARL/ARO is neither an organizer, nor provider, of any substantial logistical support for the conferences addressed in this section.

iii. Conference Support. Conference support proposals should be submitted a minimum of six (6) months prior to the date of the conference.

iv. Technical Proposal Preparation. The technical portion of a proposal for support of a conference or symposium should include:

(1) A one page or less summary indicating the objectives of the project.
(2) The topics to be covered.
(3) The location and probable date(s) and why the conference is considered appropriate at the time specified.
(4) An explanation of how the conference will relate to the research interests of the Army and how it will contribute to the enhancement and improvement of scientific, engineering, and/or educational in general and activities as outlined earlier in the research areas of this BAA.
(5) The name of chairperson(s)/(PI)(s) and his/her biographical information.
(6) A list of proposed participants and the methods of announcement or invitation.
(7) A summary of how the results of the meeting will be disseminated.
(8) A signed cover page.

v. Cost Proposal Preparation. The cost portion of the proposal should show:

(1) Total project conference costs by major cost elements.
(2) Anticipated sources of conference income and amount from each.
(3) Anticipated use of funds requested.
(4) A signed budget.

vi. Participant Support. Funds provided cannot be used for payment to any federal government employee for support, subsistence, or services in connection with the proposed conference or symposium.

vii. Cognizant ARO TPOC/ Program Manager. It is highly recommended that potential applicants contact the appropriate TPOC/ Program Manager identified earlier in the research areas of this BAA for advice and assistance before preparation of a conference/symposia proposal.

f. High School Apprenticeship Program (HSAP)/Undergraduate Research Apprenticeship Program (URAP)

i. The HSAP funds the Science, Technology, Engineering, and Mathematics (STEM) apprenticeship of promising rising high school juniors and seniors to work in a university structured research environment under the direction of ARO sponsored PIs serving as mentors. The URAP provides similar opportunities for undergraduate students. HSAP and URAP participants must be U.S. citizens or have permanent resident status. Awards will be made as add-ons to research grants, Multidisciplinary University Research Initiative (MURIs), University-Affiliated Research Contracts (UARCs), and cooperative agreements that have at least 12 months period of performance remaining from the date of HSAP/URAP proposal submission.

ii. HSAP/URAP program goals are to:

(1) Provide authentic science and engineering research experience to high school students interested in pursuing STEM, and undergraduate students pursuing science and engineering majors;
(2) Introduce students to the Army's interest and investment in science and engineering research and the associated educational opportunities available to students through the Army's Educational Outreach Program (AEOP) and DoD;
(3) Provide students with experience in developing and presenting scientific research;
(4) Provide students with experience to develop an independent research program in preparation for research fellowships, graduate school, and careers in science and engineering research;
(5) Provide opportunities for the student to benefit from the expertise of a scientist or engineer as a mentor for professional and academic development purposes; and
(6) Develop student's skills and background to prepare them for competitive entry to science and engineering undergraduate programs

iii. The HSAP/URAP is designed as an add-on to larger research projects and limited funding is available annually for PIs interested in participating. Due to the brief duration of the HSAP/URAP and limited funding we make every effort to maximize the number of student apprenticeship opportunities. PIs should submit a short proposal that clearly articulates the meaningful research that the student will conduct, along with the strategy for mentorship and facilitation of follow-on opportunities (e.g., university attendance, participation in other AEOP opportunities and other research experiences, etc). PIs must determine what aspect(s) of their current research program the student will be working on, desired deliverables, and anticipated research outcomes (based on the HSAP/URAP program goals in f. ii. of this section). PIs should describe who within their organization will be responsible for day-to-day mentoring of the students (e.g. PI, research associate, graduate student, etc.). If direct supervision of students will be someone other than the PI, the mentor's resume or curriculum vitae (CV) must be provided. The proposal should identify the gains for the student and the organization for HSAP and URAP participation in terms of technical skills, scientific reasoning in specific domains, or publication opportunities. Follow-on opportunities and relationships for students within the organization are encouraged.

Proposals should include provisions to pay HSAP students a stipend equivalent to approximately $10 per hour and URAP students a stipend equivalent to approximately $15 per hour; not to exceed 300 hours total per student. Students are not considered university employees whose hours must be tracked and therefore stipends are not required to be paid as an hourly wage but can be paid as a lump sum or divided as partial payments, at the university's discretion. Proposals should generally be limited to two students per PI, except for UARC and MURI awards on which up to 6 students are allowed. Up to four students will be considered under a single investigator if the proposal demonstrates sufficient senior research staffing to ensure effective student guidance and mentoring. Student stipends must be listed under "participant support costs" on ARO Form 99 as described in Section II.H.2.e

of this BAA.

If more than one student is proposed by a PI, there must be a near equal mix of HSAP and URAP (i.e. proposals should not be for multiple URAP students only unless approved by ARO). The institution of higher education must describe in its proposal how it will ensure the protection of minors through provision of a safe working environment.

(1) Evaluation Criteria. The evaluation criteria to be used in determining which proposals are selected for funding are described in Section II.E.1.e and II.E.2.c-d of this BAA.

(2) Describing an Outreach Strategy and Student Application Process. A primary objective of the HSAP and URAP is to expose new students to research opportunities in a research laboratory. Thus, PIs must describe a plan to attract and engage students not related to the PI (family member) or already working with the PI, laboratory, or research project. The proposal shall also include a short description (3 to 5 sentences) of the project and specific student requirements (GPA, letters of recommendation, dates of the apprenticeship, etc.). For approved proposals, the project description and requirements submitted by the PI will be marketed on the AEOP website and used in addition to the PIs outreach strategy to attract applicants. All student applications for the HSAP and URAP programs must be collected through the AEOP student application portal (www.usaeop.com). After initial AEOP eligibility screening, applications will be forward to the PI for evaluation and final candidate(s) selection. PIs must include in the proposal a plan to conduct local outreach to promote awareness of the opportunity among students/schools, and then direct them to the AEOP website to apply. HSAP/URAP is a commuter program and PIs are encouraged to perform outreach to students who are able to commute daily. PIs and mentors must also complete a brief registration annually on the AEOP website and complete a 21st Century Skills Assessment for each apprentice during the apprenticeship (web links will be emailed to the PI before the start of the summer program). At the conclusion of the apprenticeship student participants are required to develop a brief (one-page) abstract of their work to be included in an AEOP program booklet. PIs shall review and approve these abstracts before submission to ARO.

(3) Timeline. Consistent with the BAA, proposals are accepted on a rolling basis. PIs interested in receiving HSAP/URAP funding should submit proposals no later than (NLT) September 30 of the prior year to provide sufficient time for proposal review, award processing, and student outreach/recruitment. For example, to receive funding for use in summer 2020, proposals should be submitted by September 30, 2019. PIs will be notified of proposal evaluation results by mid November and student application website will open during the first week of January through the end of February.

(4) Proposal Submission. Proposals should not exceed three pages (excluding supplemental information (budget, CVs, etc.) in length and must be submitted through www.grants.gov utilizing solicitation number W911NF-17-S-0002. Complete forms Standard Form (SF) 424, ARO Form 99 (clearly distinguishing high school students from undergraduates), and upload the proposal as an attachment. Please include the title of the

research project, the grant number, and the specific number of HSAP and/or URAP opportunities requested on the first page of the proposal.

TPOC: Ms. Jennifer Ardouin, jennifer.r.ardouin.civ@mail.mil , (919) 549-4209

g. Historically Black Colleges and Universities and Minority-Serving Institutions (HBCUs/MIs)

The Army has a long history of advocating and supporting research at HBCU/MIs. Through this BAA, the CCDC's Army Research Office actively seeks proposals from the HBCU/MI community in full and open competition with all applicants. Proposals may relate to any research topic described herein. In addition to single investigator research proposals, collaborative research proposals are also encouraged. Collaborations may be between HBCU/MIs and other institutions of higher education (not limited to HBCU/MIs) and/or partners. Also included are special emphasis programs such as STIR and the YIP, described in detail elsewhere in this announcement.

TPOC: Ms. Patricia Huff, patricia.a.huff26.civ@mail.mil , (919) 549-4283

4. OTHER NON-ARO PROGRAM-RELATED INFORMATION

a. Visiting Scientist Program (VSP)

The VSP supports short-term travel opportunities for foreign/international scientists to the United States and to international conferences to socialize new S&T ideas or findings with the Army that support advancing basic research through collaboration. For additional information, contact the CCDEVCOM International Technology Center at usarmy.blenheimcrescent.rdecom.mbx.rfec-atlantic@mail.mil.

b. DoD Programs

Each year the Army Research Office, along with the Office of Naval Research (ONR) and the Air Force Office of Scientific Research (AFOSR), participates in three programs sponsored by the Office of the Assistant Secretary of Defense for Research and Engineering. These three programs, titled the Defense University Research Instrumentation Program (DURIP), MURI, and the Research and Educational Program (REP) for HBCU/MIs are conducted under separate BAAs that are posted yearly on Grants.gov and the ARO website under "Funding Opportunities". These BAAs have a definite closing date for proposal submission, and applicants are advised to review the BAAs for eligibility considerations.

For the purpose of Army funding under these three programs, the areas of interest for submitting proposals are limited to the research areas identified in this BAA.

(End of Section)