ARO Year in Review 2021

This document provides the annual historical record of the Army Research Office (ARO) programs for fiscal year 2021 (FY21), including program goals, management strategies, funding information, and key accomplishments.

Compiled and Edited by:

James A. Joseph, Ph.D.
Chapter 1
ARO Mission and Investment Strategy

The mission of the U.S. Army Combat Capabilities Development Command Army Research Laboratory’s Army Research Office focuses on creating and directing scientific discoveries 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 related to “Interactions of the Twisted Light with Quantum Systems” on page 185 (unpictured).
Message from the Director

This year the Army Research Office (ARO) Army Research Laboratory (ARL) celebrated 70 years of game-changing basic science research for warfighters. As the Army’s extramural research program, our original charter endures in our mission today to provide the foundational investments and scientific subject-matter expertise that enables critical innovation. In our long history, we have funded projects that have resulted in the highest scientific honors, including the research behind 24 Nobel Laureates. But more importantly, we have funded discoveries that have impacted the Soldier, the Army, the scientific community, and the world.

ARO traces its origin to the Office of Ordinance Research and has evolved into the Army’s foundational extramural research program. ARO became a part of the Army Research Laboratory in 1998, and we are guided by the U.S. Army Combat Capabilities Development Command (DEVCOM) and U.S. Army Futures Command (AFC). Being a part of these forward-looking organizations allows us to build a network of collaborations between academic and Army researchers, and ensures that our funded research areas align with competency-based Army research efforts to best drive scientific advances for the Soldier.

As the Army’s foundational research program, we serve as the Army’s lead interface and ambassador to the scientific community, both nationally and abroad. By engaging with the extramural community, we are able to meet people who have new ideas, invest in those ideas, and create new capabilities for the Army. We ensure that those research ideas support and drive discoveries relevant to all of the Army Modernization Priorities, Army Priority Research Areas, the greater Army, and the DEVCOM ARL Competencies.

Our programs support the whole country. We have extensive programs in outreach that encourage and enable the next generation of scientists. From high school through advanced degrees, we coordinate programs designed to foster and engage talent within science, technology, engineering, and mathematics (STEM) disciplines. We work with Historically Black Colleges and Universities and Minority-Serving Institutions providing infrastructure and incentives to improve the diversity of U.S. basic research programs and build a STEM pipeline for the Army.

As we look to the future, ARO, as a unified part of DEVCOM ARL, must adapt, identify, and pursue opportunities to generate and protect the most promising scientific discoveries that will enable Army transformation and disruptive overmatch. In order to succeed, we must do more than create and direct the right research to guide future scientific discovery; we must continually renew the network of collaborations and partnerships to benefit DEVCOM ARL, DEVCOM, AFC, the Army, and the DoD deep into the future.

The bold and far-reaching projects of the past 70 years continue to illustrate ARO’s unique ability to create synergies between basic research and transformational impact, ultimately supporting the Army’s quest to forge the future. Bringing science to the Soldier—that’s what ARO was about 70 years ago, that’s what we’re about today, and that’s what we will continue to be about 70 years from now.

Dr. Barton H. Halpern
Director, Army Research Office
DEVCOM Army Research Laboratory
Who We Are and What We Do

ARO is part of AFC DEVCOM ARL, the Army’s research laboratory. Founded in 1951 and based in Research Triangle Park, North Carolina, ARO comprises more than 100 scientists, engineers, and support staff who manage the Army’s extramural research program to create new and innovative scientific discoveries that will enable crucial capabilities and ensure technological superiority of the future Army.

ARO Mission

The mission of ARO is to create and direct scientific discoveries for revolutionary new Army capabilities, drive science to develop solutions to existing Army technology needs, accelerate the transition of basic research, educate and train the future Army scientist and engineer (S&E) workforce, create technological superiority for U.S. Forces, and prevent adversary technological surprise.

ARO serves as the Army’s principal agent for the planning, organization, selection, and management of extramural basic research in response to Army-wide requirements in the following scientific disciplines: chemical sciences, computing sciences, electronics, life sciences, materials science, mathematical sciences, mechanical sciences, network sciences, and physics. ARO utilizes the vast intellectual capital of the world’s research organizations to accomplish the following:

► Drive science to develop unprecedented Army capabilities and solutions to existing Army technology needs.
► Conceive of and exploit scientific opportunities for knowledge products.
► Leverage science and technology (S&T) to both create and prevent technological overmatch.
► Create and strengthen the partnerships among academia, industry, and government.
► Educate and train the future S&E workforce for the Army and DoD.
► Accelerate the transition of basic science research.

ARO aims to generate new scientific discoveries and innovative advances by funding high-risk, high-payoff research opportunities, principally at universities, but also with large and small businesses. These efforts support and drive the realization of the Army Functional Concepts, Essential Research Programs (ERPs); they are a critical and integral component of DEVCOM ARL Competencies. The results of these efforts are transitioned to the Army research and development community, industry, or academia to ensure technological superiority of our Soldiers, the Army, and the Nation.

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 Investment Strategy

ARO executes its mission through a long-range investment strategy designed to generate cutting-edge scientific discoveries that address the expanding range of present and future operational challenges, ultimately ensuring land force overmatch. The ARO research portfolio consists principally of foundational research efforts including Single Investigator (SI) efforts, University Affiliated Research Centers (UARCs), and specially tailored outreach programs. ARO Program Managers competitively select and fund basic science research proposals from educational institutions, nonprofit organizations, and private industry. Each program has its own objectives and set of advantages as described further in Chapter 2.

ARO’s investment strategy represents the most long-range Army view for new scientific discovery to initiate disruptive new technology, with system applications often 20-30 years away. This investment directly supports the DEVCOM ARL-wide research strategy, which is organized into 11 Competencies. Current areas of emphasis are also designated by DEVCOM ARL’s ERPs, which aim to address particular technology gaps for the current and future Army. Additionally, ARO programs and research areas are aligned with the research priorities set within the DoD: the Army Modernization Priorities, the Army Functional Concepts, and the Assistant Secretary of Defense for Research and Engineering S&T Priorities.

While the DEVCOM ARL Directorates are the primary users of the results generated through ARO’s research programs, ARO also supports research of interest for all the DEVCOM Centers, the U.S. Army Corps of Engineers (USACE), the U.S. Army Medical Research and Development Command (USAMRMC), and other Army Commands and DoD agencies. The coordination of the ARO extramural research program and joint proposal monitoring with DEVCOM ARL Directorates, DEVCOM Centers, and other Army organizations ensures a highly productive and cost-effective Army research effort.
Coordination for Program Development and Monitoring

To ensure complementary investment strategies, ARO’s extramural research programs are formulated in concert with the DEVCOM Centers and ARL-wide strategy (in addition to other Army Commands and DoD agencies). This coordination includes, but is not limited to, the following:

### DEVCOM CENTERS

- Armaments Center (DEVCOM AC)
- Army Research Laboratory (DEVCOM ARL)
- Aviation and Missile Center (DEVCOM AvMC)
- Chemical Biological Center (DEVCOM CBC)
- Command, Control, Computers Communications, Cyber, Intelligence, Surveillance and Reconnaissance Center (DEVCOM C5ISR)
- DEVCOM Analysis Center (DAC)
- Ground Vehicle Systems Center (DEVCOM GVSC)
- Soldier Center (DEVCOM SC)

### DEVCOM ARL COMPETENCIES

#### Sciences of Extreme Materials

This Competency investigates the “mechanical” response, related manufacturing methods, and performance extremes of materials, including active, adaptive, and flexible/soft materials, as well as novel manufacturing for energetic materials.

#### Humans in Complex Systems

This Competency leverages multidisciplinary, non-medical approaches to understand and modify the potential of humans situated in and interacting within complex social, technological, and socio-technical systems.

#### Electromagnetic Spectrum Sciences

This Competency aims to develop novel approaches to sensing, counter-sensing, and protection of sensing as well as testing emerging concepts for lasers, direct-energy weapons, propagation, radio frequency devices, radars, and electronic warfare.

#### Photonics, Electronics, and Quantum Sciences

This Competency studies the materials, manufacturing methods, and devices required for achieving photonic, electronic, and quantum-based effects.

#### Network, Cyber, and Computational Sciences

This Competency seeks science that enables and ensures secure resilient communication networks to facilitate distributed analytics in Multi-Domain Operations (MDO).

#### Energy Sciences

This Competency concentrates on the science of mechanical and electrical power generation storage, conditioning, and distribution, as well as energy conversion.

#### Military Information Sciences

This Competency focuses on discovering the underpinning sciences and enablers required to provide timely, mission-aware information to humans and systems at speed and scale to support all-domain and coalition operations.

#### Terminal Effects

This Competency invests in research dedicated to better understanding weapon–target interactions.

#### Mechanical Sciences

This Competency investigates the science of physical robotics and autonomy, novel mechanics, mechanisms, and control, leveraging innovations in artificial intelligence and unmanned ground and air vehicle concepts.

#### Biological and Biotechnology Sciences

This Competency explores innovative biologically related research topics, including synthetic biology, incapacitation and degradation, and augmentation.

#### Weapons Sciences

This Competency examines the science of internal, transitional, and external ballistics as well as the launch, flight, control, and navigation of guided weapons.
ARO Organizational Structure

The organizational structure of ARO mirrors the departmental structure found in many research universities. ARO's scientific Branches are aligned to a specific scientific discipline (e.g., physics), with outreach activities managed through the Technology Integration and Outreach Branch, and organization-wide support provided by the Operations and Financial Management Offices (Figure 1).

Figure 1: ARO's scientific Branches fall under the Physical Sciences, Engineering Sciences, and Information Sciences Divisions.
| **INFORMATION SCIENCES DIVISION (ISD)** | **Dr. Randy Zachery**  
Division Chief | **Mr. Tylar Temple**  
General Engineer | **Ms. Debra Brown**  
Administrative Specialist |
|---|---|---|---|
| **COMPUTING SCIENCES BRANCH** | **Dr. Purush Iyer**  
Branch Chief, Program Manager, Knowledge Systems, University Affiliated Research Centers (UARCs) | **Dr. J. Michael Coyle**  
Program Manager, Computational Architecture and Visualization | **Dr. MaryAnne Fields**  
Program Manager, Cyber Intelligent Systems |
| **MATHEMATICAL SCIENCES BRANCH** | **Dr. Joseph Myers**  
Branch Chief, Program Manager, Computational Mathematics | **Dr. Virginia Pasour**  
Program Manager, Biomathematics | **Dr. Robert Martin**  
Program Manager, Modeling of Complex Systems |
| **NETWORK SCIENCES BRANCH** | **Dr. Cliff Wang**  
Branch Chief, Program Manager, Information Assurance | **Dr. Derya Canser**  
Program Manager, Multi-Agent Network Control | **Dr. Edward Palazzolo**  
Program Manager, Social and Cognitive Networks |
| **TECHNOLOGY INTEGRATION AND OUTREACH BRANCH** | **Mr. Michael Caccuitto**  
Branch Chief | **Ms. Ivory Chaney**  
Program Manager, Education Outreach | **Ms. Nicole Fox**  
Program Manager, ARO Small Business Innovation Research (SBIR) and STTR Programs |
| **PHYSICAL SCIENCES DIVISION (PSD)** | **Dr. Lisa Troyer**  
Division Chief | **Dr. Kelby Kizer**  
Technical Assistant to the Chief | **Dr. James Burgess**  
Program Manager, UARCs: Institute for Soldier Nanotechnologies, Institute for Collaborative Biotechnologies |
| **CHEMICAL SCIENCES BRANCH** | **Dr. Hugh De Long**  
Branch Chief, Program Manager, Electrochemistry | **Dr. Elizabeth King-Doonan**  
Program Manager, Environmental Chemistry | **Dr. Dawanne Poree**  
Program Manager, Polymer Chemistry |
| **LIFE SCIENCES BRANCH** | **Dr. Micheline (Mimi) Strand**  
Branch Chief, Program Manager, Genetics | **Dr. Stephanie McElhinny**  
Program Manager, Biochemistry | **Dr. Robert Kokoska**  
Program Manager, Microbiology |
| **Dr. James Parker**  
Program Manager, Reactive Chemical Systems | **Mr. John McConville**  
Technology Transfer Officer | **Dr. Frederick Gregory**  
Program Manager, Neurophysiology of Cognition |
**CHAPTER 1**

**ARO MISSION AND INVESTMENT STRATEGY**

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Chapter 2
Program Descriptions and Funding Sources

ARO implements its investment strategy through research programs and initiatives that have unique objectives and eligibility requirements. The visions, objectives, and funding sources of these programs are presented in this chapter.

This background image is from “Thermally Drawn, Integrated Digital Fibers for Advanced Functionalities” on page 109.
Program Descriptions and Funding Sources

ARO pursues a variety of investment strategies to meet its mission to create and direct scientific discoveries for revolutionary new Army capabilities. ARO, as part of DEVCOM ARL, is a critical provider of fundamental discoveries in support of all DEVCOM ARL Competencies and ERPs. ARO implements its investment strategy through research programs and initiatives that have unique objectives and eligibility requirements. The visions, objectives, and funding sources of these programs are presented in this chapter.

The proposal topics, proposal evaluation, and project monitoring are organized within ARO Branches according to scientific discipline (refer to Chapter 1, Figure 1). Each Branch devises a research strategy and develops topics to be included in the ARO Core Broad Agency Announcement (BAA; see Appendix [online only]). Researchers are encouraged to submit white papers and proposals in areas that support a Branch’s objectives. The ARO Branches are not confined to funding research only in the academic departments that align with the Branch 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. Further, research topics that may align with more than one ARO program may be co-managed across Branches and Divisions in order to advance the interdisciplinary basic research needs of the broader scientific community.

Overview of Program Funding Sources

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

Army Funding

The Army funds the majority of the extramural basic research programs managed by ARO. These include the following:

- The ARO Core Research Program, funded through the Army’s basic research funds
- Three University Affiliated Research Centers (UARCs)
- The University Research Initiative (URI), which is overseen by the Office of the Secretary of Defense (OSD) and is divided into three component programs:
  - Multidisciplinary University Research Initiative (MURI)
  - Presidential Early Career Award for Scientists and Engineers (PECASE)
  - Defense University Research Instrumentation Program (DURIP)

ARO also participates in the Army-wide Small Business Innovation Research (SBIR) Program and manages the Small Business Technology Transfer (STTR) Program. 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.

OSD Funding

The programs managed or supported by ARO that are funded by OSD include the following:

- The Research and Educational Program (REP) for Historically Black Colleges and Universities and Minority-Serving Institutions (HBCUs/MIs)
- National Defense Science and Engineering Graduate (NDSEG) Fellowships
- High School Apprenticeship and Undergraduate Research Apprenticeship Programs (HSAP/URAP)

These activities are mandated by the DoD’s Chief Technology Office, Office of the Under Secretary of Defense for Research and Engineering [OUSD(R&E)]. ARO has been designated by OUSD(R&E) as the lead agency for the implementation of REP for HBCU/MI activities on behalf of the Tri-Service research offices—ARO, the Air Force Office of Scientific Research (AFOSR), and the Office of Naval Research (ONR).
External Funding Sources

In addition to the Army and OSD funds that directly support ARO’s mission, ARO is in the unique position to also leverage funds from other stakeholders. These funds come from a variety of sources including other Army (e.g., U.S. Army Corps of Engineers [USACE], U.S. Army Medical Research and Development Command [USAMRDC], and U.S. Special Operations Command [SOCOM]) and broader DoD (e.g., ONR, AFOSR, Defense Advanced Research Project Agency [DARPA], and Defense Threat Reduction Agency [DTRA]) organizations. While the investment strategy for leveraged funds is comparable to the investment strategy for other ARO programs, these funds often support programs with basic research needs identified by the stakeholder. As such, the external funding landscape is fluid and can change on an annual basis depending on the specific research needs of the stakeholder and technology transition opportunities made possible by ARO Program Managers (PMs).

Overview of Program Descriptions

ARO Core Research Program

The ARO Core Research Program represents the primary or “core” mechanism ARO uses to solicit and execute long-term basic research that will lead to critical new or enhanced capabilities for the future Army. Within the ARO Core Research Program, research proposals are sought from educational institutions, nonprofit organizations, and commercial organizations for basic research in the physical, engineering, and information sciences.

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. The grant awards in the SI Program typically support one or more faculty members plus graduate students and/or postdoctoral researchers for up to three years. The short grant cycle allows approximately one-third of the extramural portfolio to be reinvested into new or advancing areas each year, which provides the Army with a dynamic method for rapidly investing or divesting in research.

EARLY CAREER PROGRAM (ECP)

The objective of the ECP, formerly the Young Investigator Program (YIP), is to attract outstanding, early career university faculty to Army-relevant research questions, to support their research, and encourage their teaching and research careers. Exceptional ECP projects may be considered for the prestigious PECASE.

SHORT-TERM INNOVATIVE RESEARCH (STIR) PROGRAM

The objective of the STIR Program is to explore high-risk, 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 produces promising results, the investigator may be encouraged to submit a proposal for longer-term funding options, such as an SI Program award.

CONFERENCES, WORKSHOPS, AND SYMPOSIA SUPPORT (CF) PROGRAM

The CF Program provides funding for organizing and facilitating scientific and technical conferences, workshops, and symposia. Through this program, ARO supports and conducts 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.

RESEARCH INSTRUMENTATION (RI) PROGRAM

The 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 by providing funds to purchase instrumentation in support of new research capabilities. The RI Program represents a small percentage of the total funds ARO invests in new research capabilities, with the majority of instrumentation support awarded through the DURIP.

INTERNATIONAL PROGRAM

The International Program is part of ARO’s comprehensive approach to ensure that Army basic research funds are used to support the scientists who are best suited to drive high-risk, high-payoff Army-relevant research. The research areas that make up the International Program were identified as areas where the forerunners of the field were located in institutions outside the United States, and thus had fewer collaborative opportunities with existing Army and DoD programs. In FY20, ARO placed the management of the International Program under the Military Department (MILDEP) for unity of command. The MILDEP collaborated with the DEVCOM Forward Elements and the DEVCOM Global Technology Office to better align the international community with the Army’s basic research portfolio. Several of the ARO personnel returned in FY21 as their temporary assignment overseas concluded.
University Research Initiative (URI) Program

The URI program is managed by PMs in the Tri-Service research offices (ARO, AFOSR, and ONR), and oversight comes from the Basic Research Office of OUSD(R&E). PMs have significant flexibility and discretion in how the individual projects are monitored, while OUSD(R&E) is responsible for the overall direction.

MULTIDISCIPLINARY UNIVERSITY RESEARCH INITIATIVE (MURI) PROGRAM

The MURI program supports research efforts that require a large and highly collaborative multidisciplinary research team. This process can ultimately hasten the transition of basic research findings to practical applications and help to train students in science or engineering in areas of importance to the DoD. Therefore, the MURI program supports teams whose research efforts intersect with more than one traditional discipline. These awards are typically funded at $1.25M per year for three years with an option for two additional years. The efforts are expected to promote eventual transition to Army applications by enabling rapid research and development (R&D) breakthroughs. Selection of Army research topics and the eventual awards are reviewed and approved by OUSD(R&E) under a formal acquisition process. The full list of all ARO-managed MURI efforts that were active in FY21 are described in Chapter 4.

Eleven proposals were selected across seven MURI topics to be FY21 new starts. The corresponding MURI topic and ARO topic author(s) (and Branch) are listed, followed by the selected proposal(s), lead principal investigator (PI), and lead organization:

- **Anomalous Dipole Textures in Engineered Ferroelectric Materials**
  - ARO topic author(s)
    - Dr. Chakrapani Varanasi, Materials Science
    - Dr. Marc Ulrich, Physics
  - **Selected proposal**
    - Emergent Topological and Hierarchical Ordered Structures (ETHOS)
    - Lead PI and organization
      - Dr. Ramamoorthy Ramesh, University of California, Berkeley
  - Lead PI and organization
    - Dr. Jayakanth Ravichandran, University of Southern California

- **Cyber Autonomy through Robust Learning and Effective Human/Bot Teaming**
  - ARO topic author(s)
    - Dr. Cliff Wang, Network Sciences
    - Dr. MaryAnne Fields, Computer Sciences
  - **Selected proposal**
    - Cohesive and Robust Human–Bot Cybersecurity Teams
    - Lead PI and organization
      - Dr. Somesh Jha, University of Wisconsin–Madison
  - **Selected proposal**
    - Anomalous Polar Textures in Quasi-1D Chalcogenides and Heterostructures
    - Lead PI and organization
      - Dr. Farinaz Koushanfar, University of California, San Diego

- **Highly Heterogeneous Meta-Macrostructures Created via Fine-Particle Interactions**
  - ARO topic author(s)
    - Dr. Julia Barzyk, Mechanical Sciences;
    - Dr. Michael Bakas, Materials Science
  - **Selected proposal**
    - Understanding and Engineering Transient Mechanical Responses in Nanoparticle-Reinforced Heterogeneous Particulate Systems
    - Lead PI and organization
      - Dr. Jennifer Lewi, Harvard University

- **The Same is Different: Integrating Multiple Phenomena in Single Materials**
  - ARO topic author(s)
    - Dr. Marc Ulrich, Physics
    - Dr. Chakrapani Varanasi, Materials Science
  - **Selected proposal**
    - Multifunctional Devices in Precisely Engineered van der Waals Homojunctions
    - Lead PI and organization
      - Dr. Philip Kim, Harvard University

- **Quantum Network Science**
  - ARO topic author(s)
    - Dr. Derya Cansever, Network Sciences
  - **Selected proposal**
    - Theory and Engineering of Large-Scale Distributed Entanglement
    - Lead PI and organization
      - Dr. Saikat Guha, University of Arizona
  - **Selected proposal**
    - Robust Entanglement Distribution in Quantum Networks – Network Science and Architectures for Novel Quantum Information Processing
    - Lead PI and organization
      - Dr. Chee Wei Wong, University California, Los Angeles

- **Tunable Dilute Anion III-Nitride Nanostructures for Stable Photocatalysis**
  - ARO topic author(s)
    - Dr. Hugh DeLong, Chemical Sciences
  - **Selected proposal**
    - Tunable III-Nitride Nanostructures for N=N and C–H Bond Activation
    - Lead PI and organization
      - Dr. Zetian Mi, University of Michigan
The following seven topics were selected in FY20 and constitute the ARO portion of the FY22 MURI BAA. The corresponding ARO PM authors (and Branch) are also listed:

**Bio-architected Responsive Materials with 3D Nanoscale Order**
ARO topic author(s)
Dr. Stephanie McElhinny, Life Sciences
Dr. Evan Runnerstrom, Materials Science

**Irregular Metamaterial Networks**
ARO topic author(s)
Dr. Daniel Cole, Materials Science
Dr. Derya Cansever, Network Sciences

**Gut-Neuronal Signaling Through Polymeric Mucin via Chemical Probes and Imaging**
ARO topic author(s)
Dr. Dawanne Poree, Chemical Sciences
Dr. Robert Kokoska, Life Sciences

**Topological Seeds of Complex Response in Materials**
ARO topic author(s)
Dr. Joseph Myers, Mathematical Sciences
Dr. Daniel Cole, Materials Science

**Uncovering the Underlying Neurobiological Mechanisms of Cognitive Fatigue**
ARO topic author(s)
Dr. Virginia Pasour, Mathematical Sciences
Dr. Frederick Gregory, Life Sciences

**ELECTROBIOLOGY: Electronic Control of Biological Communication**
ARO topic author(s)
Dr. Albena Ivanisevic, Electronics
Dr. Micheline (Mimi) Strand, Life Sciences

**Connectivity and Transport in Disordered Hyperuniform Networks**
ARO topic author(s)
Dr. Evan Runnerstrom, Materials Science
Dr. Robert Ulman, Network Sciences

**DEFENSE UNIVERSITY RESEARCH INSTRUMENTATION PROGRAM (DURIP)**

The DURIP supports the purchase of equipment that augments current university capabilities or develops new capabilities to achieve cutting-edge defense research. In FY21, the Army awarded 38 grants totaling $8.6M, with an average award of $227K.

**University Affiliated Research Centers (UARCs)**

The UARCs are strategic, Army-sponsored, DoD-designated research organizations at universities. The UARCs were formally established in May 1996 by OUSD(R&E) to advance DoD long-term goals by pursuing cutting-edge basic research and maintaining core competencies in specific domains beneficial to the DoD. Collaborations among the UARCs and the educational and research resources available at the associated universities can enhance the ability of the UARCs to meet the long-term goals of the DoD.

ARO is the primary sponsor for two UARCs and co-manages a third:
The Institute for Soldier Nanotechnologies (ISN), located at the Massachusetts Institute of Technology (MIT)

The Institute for Collaborative Biotechnologies (ICB), located at the University of California, Santa Barbara, with MIT and the California Institute of Technology (Caltech) as academic partners

The 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 DEVCOM SC, where ARO is responsible for managing basic research efforts and DEVCOM SC is responsible for managing applied efforts.

**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 purpose of these programs is to (1) stimulate technology innovation, (2) use small business to meet federal R&D needs, (3) foster and encourage participation by socially and economically disadvantaged small business concerns 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 businesses must partner with universities, federally funded R&D centers, or other nonprofit research institutions to develop and transition ideas from the laboratory to the marketplace.

The SBIR and STTR Programs are overseen by OUSD(R&E). Numerous organizations participate in the DoD’s SBIR Program including the Army, Navy, Air Force, DARPA, SOCOM, DTRA, Missile Defense Agency (MDA), National Geospatial Intelligence Agency (NGA), and Chemical Biological Defense Program (CBD). The Army-wide SBIR Program is managed at DEVCOM Headquarters, which enables ARO to participate in both the Army-wide SBIR Program as well as SBIR Programs supported by other organizations across the DoD. The Army-wide STTR Program is managed by ARO. The STTR Program at ARO coordinates participation of nine Army Components and Commands, and invests in all Army Modernization Priorities. In addition to DEVCOM ARL participation through ARO, other participating components include DEVCOM AvMC, DEVCOM AC, DEVCOM CSISR, DEVCOM CBC, DEVCOM SC, DEVCOM GVSC, USACE, and USAMRDC.

Each year, the SBIR and STTR Programs develop a set of topics that represent the DoD’s anticipated technology needs. Subject-matter experts at ARO often participate in this process by developing topics for publication in the DoD SBIR and STTR BAAs. Small businesses can then submit proposals to specific topics listed in the BAAs, which are competitively selected for funding. The SBIR and STTR Programs fund proposals through a three-phase process. Phase I is the point of entry into the program and involves a feasibility study that determines the scientific, technical, and commercial merit and feasibility of a concept. Phase II represents a major R&D effort, culminating in a well-defined deliverable prototype (i.e., a technology, product, or service). Phase II awardees are competitively selected from Phase I awardees who submitted a Phase II proposal. Phase II awardees may then be selected to receive additional funds as an invited Subsequent Phase II or Phase II Enhancement (SBIR only), or via the Commercialization Readiness Program (SBIR only). Phase III represents the commercialization of the product.

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.

**ARO FY21 SBIR TOPICS**

The lead topic author (who serves as the topic PM) and corresponding Branch are listed with each topic:

- Direct Wall Shear Stress Measurement for Rotor Blades, Matthew Munson, Mechanical Sciences
- Augmented Reality CBRN Threat Display for Mounted Situational Awareness, Dawanne Poree, Chemical Sciences
- Electronically-Tunable, Low Loss Microwave Thin-Film Ferroelectric Phase-Shifter, Joe Qiu, Electronics
- Field Portable Bioaerosol Identification via Mass Spectrometry, Elizabeth King-Doonan, Chemical Sciences
ARO FY21 STTR TOPICS

The lead topic author (who serves as the topic PM) and corresponding Branch are listed with each topic:

► A Revolutionary RF Circuit Simulator for New Electronic Design and Analysis Capabilities, Tylar Temple, Information Sciences
► 300W Low-Temperature SOFC Army Power Sources, Rob Mantz, Engineering Sciences
► Photonic Accelerators for Artificial Neural Networks, Mike Gerhold, Electronics
► Cryo-CMOS Integrated Circuits, Joe Qiu, Electronics
► Virtual Off-Road Simulator for Teams of Bots and Autonomous/Conventional Wheeled/Tracked Vehicles, Joe Myers, Mathematical Sciences
► Actuation for Human-Scale Dynamic Whole-Body Manipulation, Joe Myers, Mathematical Sciences
► Physical Monitoring Techniques to Improve Warfighter Performance, Fred Gregory, Life Sciences
► Three-Dimensional Microfabricated Ion Traps for Quantum Sensing and Information Processing, Sara Gamble, Physics
► Additive Manufacturing of Thermally Cured Thermostet Polymers, Dawanne Poree, Chemical Sciences
► Cost Effective Synthesis of Linear Ring Opening Metathesis Polymers, Dawanne Poree, Chemical Sciences
► Reducing COVID-19 Mortality by Reducing Post-Hyperimmunity Period Immune Suppression, Mimi Strand, Life Sciences

ARO FY21 SBIR PHASE II CONTRACT AWARDS

The lead topic author and corresponding Branch are listed following each topic title:

► Non-LOS Directional Command and Control, Stephen Lee, Army Research Office
► New Concept for a Low Distortion, High-Power, High-Efficiency mm-Wave RF Power Amplifier Circuit, Tylar Temple, Information Sciences
► Canine Non-LOS Directional Control System, Stephen Lee, Army Research Office
► Field Deployable Kit for Removal of Aromatic Hydrocarbon and Heavy Metal Contaminants from Firefighter Turnout Gear, Dawanne Poree, Chemical Sciences
► On-site Electro-synthesis of Potassium Formate from Recycled CO₂ – Phase II, Hugh DeLong, Chemical Sciences

ARO FY21 STTR PHASE II CONTRACT AWARDS

The lead topic author and corresponding Branch are listed following each topic title:

► A Wideband Transmitter Based on Signal Segmentation, Joe Myers, Mathematical Sciences
► Tunable Active HEterodyne Terahertz Imaging (TAHEtI), Joe Qiu, Electronics
► Solid Oxide Fuel Cell Generator, Rob Mantz, Engineering Sciences
► Man-Portable, Direct-Fuel Capable, Tubular Solid Oxide Fuel Cell, Rob Mantz, Engineering Sciences
► Multi-Hit Performance of Small Arms Protective Armor, Dan Cole, Materials Science
► Mitigation of Ransomware, Cliff Wang, Network Sciences
► Throughput Optimization for the Tailorable Universal Feedstock for Forming (TuFF) Process, Michael Bakas, Materials Science
► Diamond Electron Amplifiers, Joe Qiu, Electronics
► Tunable, High-Speed, Resonant-Cavity Infrared Detectors and Narrow-Linewidth Quantum Cascade Lasers for Free-Space Communication Links, Mike Gerhold, Electronics
► Isogeometric Analysis Methods for High Fidelity Mobility Applications, Joe Myers, Mathematical Sciences
► Low Temperature Atomic Layer Deposition of Manganese Telluride on Topological Insulator, Marc Ulrich, Electronics
► Exploiting Single Nucleotide Polymorphisms for Extreme Performance, Mimi Strand, Life Sciences
► Intrinsically Interference and Jamming-Resistant High Frequency (HF) Radios, Joe Qiu, Electronics
► Millimeter Waveforms for Tactical Networking, Bob Ulman, Network Sciences
► Position, Navigation and Timing (PNT) Without the Global Positioning System (GPS), Derya Cansever, Network Sciences
► Tactical Edge Sensor Processing – Edge Learning System Orchestration and Management, Derya Cansever, Network Sciences
ARO FY21 SBIR PHASE III CONTRACT AWARDS

The lead topic author and corresponding Branch are listed following each topic title:

- IDIQ for USASOC Engineering Analysis and Support, Stephen Lee, Army Research Office
- POSS® Viscoelastic Hemostat, Rob Mantz, Engineering Sciences
- Development of Comprehensive Biothreat Identifier – Zeteo Threat Agent Detection System (zTADS), Dawanne Poree, Chemical Sciences
- Electromagnetically Catalyzed Decontamination (EMCAT) Development, Stephen Lee, Army Research Office
- Artificial Intelligence (AI) for Tactical Power, Operations and Advanced Manufacturing, Stephen Lee, Army Research Office

ARO FY21 STTR PHASE III CONTRACT AWARDS

The lead topic author and corresponding Branch are listed following each topic title:

- Modeling of Complex Systems, Dr. Robert Martin, Mathematical Sciences
- Biomathematics, Dr. Virginia Pasour, Mathematical Sciences
- Solid Mechanics, Dr. Denise Ford, Mechanical Sciences
- Environmental Chemistry, Dr. Elizabeth King-Doonan, Chemical Sciences
- Electronic Sensing, Dr. Tania Paskova, Electronics

Defense Established Program to Stimulate Competitive Research (DEPSCoR)

As part of the FY21 defense appropriations bill, Congress tasked the Basic Research Office with managing the Defense Established Program to Stimulate Competitive Research (DEPSCoR). DEPSCoR is a capacity-building program designed to strengthen the research infrastructure at institutions of higher education in underutilized states/territories.

The authorization legislation for DEPSCoR included a formula to determine which states/territories are eligible for the program based on the level of DoD science and engineering R&D funds that were obligated to institutions of higher education within a state/territory over a three-year average. Thirty-four states, the Commonwealth of Puerto Rico, Guam, and the U.S. Virgin Islands were eligible to participate in FY21 DEPSCoR (Figure 1).

The Basic Research Office anticipates approximately $12.6 million in total funding will be made available to fund approximately 21 awards up to $600,000 (total cost) each. Each award will be funded up to $200,000 (total cost) per year for three years in the form of a grant. The awards will be made across the Services, with five of those awards expected to be made to ARO-led topics.

The lead topic author and corresponding Branch are listed with each topic:

- Modeling of Complex Systems, Dr. Robert Martin, Mathematical Sciences
- Solid Mechanics, Dr. Denise Ford, Mechanical Sciences
- Electronic Sensing, Dr. Tania Paskova, Electronics

To meet the directives outlined by Congress, the Basic Research Office hosted a virtual DEPSCoR Day on Wednesday, 23 June 2021, in which ARO participated. The event served to raise awareness of the Basic Research enterprise, encouraged increased participation in the DoD’s initiatives to support national security functions, and facilitated dialogue between Program Managers and attendees.
Historically Black Colleges and Universities and Minority-Serving Institutions (HBCU/MI) Program

ARO (CORE) HBCUs/MIs PROGRAM

Academic institutions classified as HBCUs/MIs may submit proposals to the core ARO BAA, as for any other institutions, and are evaluated and selected according to the same evaluation criteria and process established for all proposal submissions to the ARO Core Research Program BAA. In FY20, ARO supported 104 agreements with HBCUs/MIs—30 of which were new agreements in FY21—receiving over $25.3M in FY21 funding.

In FY21, ARO funded 3 HBCU/MI Research Centers of Excellence, a first time effort. The focus of the HBCU/MI Research Centers of Excellence Program is to advance innovative basic research leading to potential technology development in areas of strategic importance to the Army. Awards have five-year periods of performance, with one each in the information, engineering, and physical sciences, supporting Army, AFC and DEVCOM goals to broaden the performer base and diversify the research ecosystem. Centers were competitively selected and awarded to the University of the District of Columbia (HBCU), Florida International University (MI), and University of Illinois Chicago (MI). FY21 investments in this new initiative totaled $1.3M ($446K for 1 HBCU; $931K for 2 MIs). Listed below are the new Centers of Excellence:

► Center of Excellence for Acoustic and Seismic Sensing of Urban Environments at the University of the District of Columbia, Professor Max Denis, University of the District of Columbia; Dr. Julia Barzyk, Materials Science (Competencies: Mechanical Sciences; Military Information Sciences)

► FINDS Research Center: The Forensic Investigations Network in Digital Sciences (FINDS) Research Center: A Proposal for Development of Advanced Digital Forensic Research by Networked HBCU/MSIs for The Department of Defense, Professor Sundararaj Iyengar, Florida International University; Dr. Cliff Wang, Network Sciences (Competencies: Military Information Sciences; Network, Cyber, and Computational Sciences)

► A Multidisciplinary Research Center of Excellence – EXEED, Professor Russell Hemley, University of Illinois Chicago; Dr. James Parker, Chemical Sciences (Competencies: Sciences of Extreme Materials)

► Transformational HPC System based on Field Programmable Gate Arrays Tailored for Simulations and Machine Learning of Transonic Laminar-Turbulent Transition, Professor Hermann Fasel, University of Arizona; Dr. Ralph Anthenien, Mechanical Sciences (Competencies: Mechanical Sciences; Network, Cyber, and Computational Sciences; Weapons Sciences)

► Massive MIMO and Millimeter-wave Integrated Tactical Communication for Swarm Networks: Design and Experiment, Professor Tadilo Bogale, North Carolina Agricultural and Technical (A&T) State University; Dr. Derya Cansever, Network Sciences (Competencies: Mechanical Sciences; Military Information Sciences; Network, Cyber, and Computational Sciences)

► Equipment Support for Cloud-Based Intelligent VR Systems, Professor Ming Lin, University of Maryland, College Park; Dr. Michael Coyle, Computing Sciences (Competencies: Mechanical Sciences; Network, Cyber, and Computational Sciences)

► A Millimeter-Wave Communication System for Wireless Security and Networking Research and Education, Professor Ming Li, University of Arizona; Dr. Cliff Wang, Network Sciences (Competencies: Network, Cyber, and Computational Sciences)

► Redox Reactions of Chromium, Copper, and Iron Mixtures in Contaminated Waters: Integration of Laboratory Experiments, Reactive Transport Modeling, Spectroscopy, and Electrochemical Sensing, Professor José Cerrato, University of New Mexico; Dr. Elizabeth King-Doonan, Chemical Sciences (Competencies: Biological and Biotechnology Sciences; Energy Sciences)

► Human-Guided Online Learning for Long-Term Autonomy with Active Self Evaluation, Professor Yongcan Cao, University of Texas at San Antonio; Dr. Maryanne Fields, Computing Sciences (Competencies: Humans in Complex Systems; Military Information Sciences)

► Floating-Point Photonic Accelerators, Professor Guifang Li, University of Central Florida; Dr. Michael Gerhold, Electronics (Competencies: Photonics, Electronics, and Quantum Sciences; Military Information Sciences; Network, Cyber, and Computational Sciences)

► 2021-2022 ARO-HU Interdisciplinary STEM Conference on Mathematical Biology: Modeling and Analysis, Professor Abdul-Aziz Yakubu, Howard University; Dr. Virginia Pasour, Mathematical Sciences (Competencies: Biological and Biotechnology Sciences; Humans in Complex Systems)
1. **Knowing the Unknown: Exploring the Space of Adversarial Attacks via Causal Learning**, Professor Huan Liu, Arizona State University; Dr. Purush Iyer, Computing Sciences (Competencies: Military Information Sciences; Network, Cyber, and Computational Sciences)

2. **Dataflow-Based Design for Real-Time Scene Understanding at the Edge**, Professor Shuvra Bhattacharyya, University of Maryland, College Park; Dr. Maryanne Fields, Computing Sciences (Competencies: Military Information Sciences)

3. **Mech-DEFECT: Mechanically-Induced Defect Equilibria for Engineered Complexion Transitions**, Professor Timothy Rupert, University of California, Irvine; Dr. Denise Ford, Mechanical Sciences (Competencies: Sciences of Extreme Materials)

4. **Enabling Solid-State Quantum Sensors with Reduced SWaP for DoD Applications**, Professor Ronald Walsworth, University of Maryland, College Park; Dr. Paul Baker, Physics (Competencies: Photonics, Electronics, and Quantum Sciences)

5. **Environmental Impact on Explosives Detection Dogs and Mitigation Strategies – Research in Physical Sciences**, Professor Paola Tiedemann, Texas Technical University; Dr. Stephen Lee, ARO Senior Research Scientist (Competencies: Biological and Biotechnology Sciences)

6. **A Geometric Approach to Explainable Machine Learning**, Professor Ying-Cheng Lai, Arizona State University; Dr. MaryAnne Fields, Computing Sciences (Competencies: Mechanical Sciences)

7. **Stacking and Twisting van der Waals Heterostructures for Ultrafast and Ultrasensitive Vibronic Sensors**, Professor Nathaniel Gabor, University of California, Riverside; Dr. Tania Paskova, Electronics (Competencies: Photonics, Electronics, and Quantum Sciences)

8. **Unraveling Tethered Protein Interfacial Assembly Dynamics: Multimodal Optical and Electrochemical In-Situ Investigations of Reflectin**, Professor Daniel Morse, University of California, Santa Barbara; Dr. Stephanie McElhinny, Life Sciences (Competencies: Biological and Biotechnology Sciences)

9. **Data-DRiven Online Scalable Situation Learning (DDROSSIL)**, Professor Ioannis Schizas, University of Texas at Arlington; Dr. Robert Martin, Mathematical Sciences (Competencies: Humans in Complex Systems)

10. **Logic and Geometry in Quantum Computing**, Professor John Harding, New Mexico State University; Dr. Joseph Myers, Mathematical Sciences (Competencies: Photonics, Electronics, and Quantum Sciences)

11. **Free-Space Optical Communication in Plasma Waveguides**, Professor S. Rostami Fairchild, University of Central Florida; Dr. James Joseph, Physics Branch (Competencies: Energy Sciences)

12. **DNA-Accelerated Radical Polymerization**, Professor Peng He, North Carolina A&T State University; Dr. Dawanne Poree, Chemical Sciences (Competencies: Biological and Biotechnology Sciences)

13. **Electrical Conductivity of Graphite**, Professor Manfred Wuttig, University of Maryland, College Park; Dr. Pani Varanasi, Mechanical Sciences (Competencies: Electromagnetic Spectrum Sciences; Energy Sciences; Photonics, Electronics, and Quantum Sciences)

14. **Gradient Nano-Structures from Dissipative Nonequilibrium Self-Assembly of Block Copolymers**, Professor Xiao Li, University of North Texas; Dr. Evan Runnerstrom, Mechanical Sciences (Competencies: Photonics, Electronics, and Quantum Sciences; Sciences of Extreme Materials)

15. **COVERT ID: Cybersecurity Operations Vectors: Verifying External Resilience of Transgressors and their Identification through Cybersecurity Forensics**, Professor Sundararaj Iyengar, Florida International University; Dr. Cliff Wang, Network Sciences (Competencies: Network, Cyber, and Computational Sciences)

16. **Revealing and Tailoring Mechanical Behaviors of Multi-Principal Element Alloys under Extreme Thermomechanical Conditions**, Professor Penghui Cao, University of California, Irvine; Dr. Daniel Cole, Mechanical Sciences (Competencies: Mechanical Sciences; Sciences of Extreme Materials; Weapons Sciences)

17. **A New High-Order Accurate Approach for Modeling of Wave Propagation and Heat Transfer in Heterogeneous Materials**, Professor Alexander Idesman, Texas Technical University; Dr. Daniel Cole, Mechanical Sciences (Competencies: Mechanical Sciences; Sciences of Extreme Materials)

18. **Matrix-Assisted Laser Desorption Ionization Mass Spectrometer and Size Exclusion Chromatographer to Characterize Metal-Chelating and Self-Healing Polymers**, Professor Marco Giles, Prairie View A&M University; Dr. Dawanne Poree, Chemical Sciences (Competencies: Science of Extreme Materials)

19. **Real-Time Deconvolution of Complex Chemical Matrices**, Professor Suchol Savagatrup, University of Arizona; Dr. Elizabeth King-Doonan, Chemical Sciences (Competencies: Biological and Biotechnology Sciences; Photonics, Electronics, and Quantum Sciences)
PARTNERED RESEARCH INITIATIVE (PRI) PROGRAM

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 HBCUs/MIs research teams into existing DEVCOM 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 FY21, DEVCOM ARL’s PRI Program for HBCUs/MIs concluded.

The CRA and CTA program and PRI topics are listed, with the lead PI, collaborating institution, and cooperative agreement manager (CAM) also listed for each topic:

Cyber Security CRA

**PRI Topic**
Defeating the Dark Triad in Cybersecurity Using Game Theory Integrated into Cybersecurity

**Lead PI and organization**
Dr. Christopher Kiekintveld, University of Texas at El Paso

**CAM**
Dr. Michael Frame

Materials in Extreme Dynamic Environments (MEDE) CRA

**PRI Topic**
Tailoring Mg-Alloy Systems through Composition/Microstructure/Severe Plastic Deformation for Army Extreme Dynamic Environment Applications

**Lead PI and organization**
Dr. Jagannathan Sankar, North Carolina A&T State University

**CAM**
Dr. Sikhanda Satapathy

Multiscale Modeling of Electronic Materials (MSME) CRA

**PRI Topic**
Material Design Under Uncertainty

**Lead PI and organization**
Dr. Yanyan He, New Mexico Institute of Mining and Technology

**CAM**
Dr. Meredith Reed

Cognition and Neuroergonomics (CaN) CTA

**PRI Topic**
Reliability of Neural Activity as an Assay of Cognitive State

**Lead PI and organization**
Dr. Jacek Dmochowski, The City College of New York

**CAM**
Dr. Jon Touryan

DOD RESEARCH AND EDUCATIONAL PROGRAM (REP) FOR HBCUS/MIS

ARO has administered the REP on behalf of OUSD(R&E) since 1992. Under this program, qualifying institutions are able to submit proposals to compete for basic research and equipment grants. The REP aims to enhance research capabilities of HBCUs and MIs and strengthen their education programs in science, technology, engineering, and mathematics (STEM) disciplines that are relevant to the defense mission.

In FY21, 70 equipment grants totaling $30.4M were made to 25 unique HBCUs, 31 unique MIs, and one Tribal college.

Education Outreach Program

NATIONAL DEFENSE SCIENCE AND ENGINEERING GRADUATE (NDSEG) FELLOWSHIP PROGRAM

The DoD NDSEG Fellowship Program is a Tri-Service research office (ARO, AFOSR, ONR) program administered by AFOSR, designed to increase the number of U.S. citizens trained in disciplines of science and engineering important to defense goals. 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 intend to pursue a doctoral degree in a scientific discipline of interest to the military. The NDSEG Fellowship lasts for three years and provides full tuition, a monthly stipend, a travel budget for professional development, and health insurance.

NDSEG Fellows are selected following a merit-based evaluation of the applicant’s academic records, recommendations, GRE scores, and technical applications. ARO PMs serve as reviewers for applications and mentors for selectees in their areas of expertise.

In FY21, ARO selected 53 NDSEG Fellows, who began their fellowships in fall 2021.
CHAPTER 2  
PROGRAM DESCRIPTIONS AND FUNDING SOURCES

- **Aarti Mathur**, Chemical Engineering  
  Investigations of Model Interfaces as a Function of Reaction Conditions in MIS Water Splitting Devices, University of Michigan

- **Andrea Boskovic**, Computer and Computational Sciences  
  Novel Techniques for Positive Unlabeled Learning in Anomaly Detection, University of Washington

- **Andrew Curtis**, Mechanical Engineering  
  Passive Target Tracking via Mobile-Node Distributed Sensor Networks, Northwestern University

- **Arjun Desai**, Biomedical Engineering  
  Personalized Risk Assessment of Post-Traumatic Early Knee Osteoarthritis Using a Low-Cost, Rapid, and Multi-Modal Imaging and Biomechanics Approach, Stanford University

- **Ashley Ogorek**, Chemistry  
  A DNA Nanocatalyst for Abiotic Analyte-Responsive Gene Control, University of Wisconsin–Madison

- **Benjamin Kruse**, Chemistry  
  Olympic Gel Synthesis and Molecular Dynamics Modeling to Probe Entanglements for Elastomer Toughening, University of North Carolina at Chapel Hill

- **Brandon Chen**, Biosciences (including Toxicology)  
  Metabolic Regulation of ER-Mitochondrial Contacts, University of Michigan

- **Brandon Desousa**, Biosciences (including Toxicology)  
  Hypoxia Stabilization of Complex I as a Therapy for Primary and Secondary Mitochondrial Dysfunction, Rutgers University

- **Brian Wyatt**, Mechanical Engineering  
  Compositional and Structural Control of the Mechanical Properties of Two-Dimensional Transition Metal Carbides and Nitrides, Indiana University–Purdue University Indianapolis

- **Camille Phaneuf**, Cognitive, Neural, and Behavioral Sciences  
  Behaviorally and Neu rally Characterizing How Actionable Information Is Valued Under Different Cognitive Demands, Harvard University

- **Christopher Dade**, Chemistry  
  Disarming Drug Resistance: Identifying Inhibitors of the Integral Membrane Aspartic acid Protease PilD that are Anti-Infective Drug Leads to Treat Pseudomonas Aeruginosa Infections, University of Wisconsin–Madison

- **Christopher Jackson**, Civil Engineering  
  Blast Characterization of Metal Alloys Dispersed by Hydrocarbon Detonations, Virginia Polytechnic Institute and State University

- **Donald Hejna**, Computer and Computational Sciences  
  Morphological Generalization for Efficient Learning, Stanford University

- **Edward Chen**, Computer and Computational Sciences  
  Ultrasound Anywhere, Anytime: Artificial Intelligence for Unforeseen Variations in Ultrasound Imaging, Stanford University

- **Ethan Fahnestock**, Computer and Computational Sciences  
  Steps toward Improving Manned-Unmanned Teaming: Language-Guided Reactive Perception with Bayesian Reasoning for Mobile Manipulators, Massachusetts Institute of Technology, Woods Hole Oceanographic Institution (WHOI)

- **Gabriella Muwanga**, Biomedical Engineering  
  Using Ultrasound-Responsive Uncaging of Drug-Loaded Nanoparticles to Study Neuro-Glial Interplay in Adrenergic Receptor-Associated Analgesia in a Mouse Model of Post Injury Pain, Stanford University

- **Gautam Bordia**, Materials Science and Engineering  
  Towards the Rational Design of Functional All-Liquid Materials, University of California, Berkeley

- **Grace Hu**, Materials Science and Engineering  
  Computational Design of Low-Cost, 4D-Printed Shape Transforming Metamaterials, University of California, Berkeley

- **Hamza Raniwala**, Physics (including Optics)  
  Efficient Superconductor-to-Spin Transducer for Hybrid Quantum Computing, Massachusetts Institute of Technology

- **Heidi Myers**, Geosciences (including Terrain, Water, and Air)  
  Development of an Aerial Vehicle (AVAILD) using Artificial Intelligence for Landmine Detection, University of Maryland, College Park

- **Helen Sakharova**, Biosciences (including Toxicology)  
  Rules for Synonymous Codon Choice: When Do Clusters of Suboptimal Codons Matter?, University of California, Berkeley

- **Henry Love**, Electrical Engineering  
  A Highly Digital, Low-Power Optical Analog-to-Digital Converter, University of Pennsylvania

- **Hersh Bhargava**, Biomedical Engineering  
  Programmable Spatial Targeting of Designer Immune Cells through in Silico Modeling and In Vivo Characterization, University of California, San Francisco

- **Jack-William Barotte**, Mathematics  
  Meltwater Production in Temperate Zones, Brown University

- **Jacob Elkins**, Aeronautical and Astronautical Engineering  
  (including Space Physics)  
  Adaptive Online Learning Systems via Distributed Reinforcement Learning, University of Alabama in Huntsville

- **Jacob Vagott**, Materials Science and Engineering  
  ALD/MLD of 2D Halide Perovskite Thin Films for High-Performance X-Ray Detectors, Georgia Institute of Technology

- **Jaelyn Bos**, Biosciences (including Toxicology)  
  Modeling a Complex Coastal Ecosystem with a Spatially Explicit Approach, Temple University

- **Javier Morales Ferrer**, Mechanical Engineering  
  4D Printing Materials with Programmed Responsiveness and Stiffness for Multifunctional Architectures, Boston University
► Jerika Chiong, Chemistry
Next-Generation Degradable Electronics for Security, Defense, and Combat Casualty Care, Stanford University

► Joshua Lederman, Electrical Engineering
A Novel Photonic/FPGA Integrated System for Accelerated Low-Power Neuromorphic AI Image Processing, Princeton University

► Justin Bui, Chemical Engineering
Electrochemical Synthesis of Ammonia via Membrane-Electrode Assemblies Containing Distinct Solvent and pH Microenvironments, University of California, Berkeley

► Katarina Heyden, Biosciences (including Toxicology)
Molecular Mechanisms Underlying Adverse Effects of Excess Folic Acid Exposure, Cornell University

► Kelsey Hern, Biomedical Engineering
Developing a Deep Learning Framework for Informing Phage Therapy for Treatment of Wound Infections, University of California, Berkeley

► Kelsey Neuenswander, Cognitive, Neural, and Behavioral Sciences
Threat Detection in Vocal Ensembles, University of California, Los Angeles

► Matthew Asper, Aeronautical and Astronautical Engineering (including Space Physics)
Electromechanical Modeling and Testing of a Novel Electrically Driven Coaxial Rotor System, University of Texas at Austin

► Montana Minnis, Chemical Engineering
Stacking-Frustrated Assemblies of Shape-Controlled Microparticles, University of Colorado Boulder

► Natalie Mueller, Biomedical Engineering
Mechanically-Adaptive, Resveratrol-Eluting Probe to Mitigate Intracortical Microelectrode Failure for Neuromusculoskeletal and Spinal Cord Injury Rehabilitation Applications, Case Western Reserve University

► Nicholas Lauersdorf, Materials Science and Engineering
Programmable Multi-Component Active Matter, University of North Carolina at Chapel Hill

► Nikhil Shinde, Computer and Computational Sciences
Safe, Intelligent, Context Aware Decision Making for Surgical Robot Automation, University of California, San Diego

► Noël Brindise, Aeronautical and Astronautical Engineering (including Space Physics)
xAI as Translation: Towards Human-Oriented Explanation of Artificially Intelligent Aerospace Systems, University of Illinois at Urbana-Champaign

► Samantha Lauro, Chemistry
Optimization of Battery Energy Density through Substrate-Free Electrode Design, University of Texas at Austin

► Seth Temple, Mathematics
Methods in Statistical Genetics to Study Natural Selection in Humans, University of Washington

► Shreyas Parthasarathy, Physics (including Optics)
Quantum Decoherence Probe Station for Studying and Mitigating Decoherence at Interfaces in Qubit Platforms, University of California, Santa Barbara

► Simon Evered, Physics (including Optics)
Highly Entangled Quantum Matter in Programmable, Three-Dimensional Atom Arrays: Generation, Probing, and Applications, Harvard University

► Stephanie Williams, Cognitive, Neural, And Behavioral Sciences
Driving CSF Clearance of Solutes during the Wake State to Optimize Brain Health, Boston University

► Theo Diamandis, Computer and Computational Sciences
Collaborative Learning with Diverse Data, Massachusetts Institute of Technology

► Theodore Letsou, Electrical Engineering
Infrared Quantum Cascade Laser Frequency Combs for Chemical Detection in Dual-Comb Spectrometer, Massachusetts Institute of Technology

► Travis Leadbetter, Mechanical Engineering
Discovering Far From Equilibrium Models by Leveraging Fluctuations of Macroscopic Observables, University of Pennsylvania

► Tyler LaBonte, Computer and Computational Sciences
Reconciling Theory and Practice for Trusted Deep Learning: Compositional Regularization in Double Descent, Georgia Institute of Technology

► Vladislav Sevostianov, Geosciences (including Terrain, Water, and Air)
Advancing Human Capabilities in Smell, Princeton University

► Yihua Zhong, Physics (including Optics)
The Non-Equilibrium Statistical Mechanics of Metabolism, University of California, Berkeley

► Zachary Stein, Aeronautical and Astronautical Engineering (including Space Physics)
Lifetime Predictions of Alternative Particulate-Infiltrated High Temperature Coatings, University of Central Florida
HIGH SCHOOL APPRENTICESHIP PROGRAM (HSAP) AND UNDERGRADUATE RESEARCH APPRENTICESHIP PROGRAM (URAP)

The HSAP and URAP are managed by the Army Education Outreach Program (AEOP) Outreach Office at DEVCOM Headquarters and administered by ARO.

The HSAP funds the STEM apprenticeships of promising high school juniors and seniors to work in university-structured research environments under the mentorship of ARO-sponsored PIs or their senior research staff. In FY21, HSAP awards provided 36 students with research experiences at 19 universities in 12 states. Seven of the universities were HBCUs/MIs. ARO invested approximately $46K into the FY21 HSAP effort, and the AEOP contributed matching funds.

The URAP funds STEM apprenticeship of undergraduates to work in research groups under the mentorship of ARO-sponsored PIs or their senior research staff. In FY21, URAP awards provided 62 students with research experiences at 35 universities in 18 states. Nine of the universities were HBCUs/MIs. ARO invested approximately $206K into the FY21 URAP effort, and the AEOP contributed matching funds.

For a peek into the AEOP Program, check out the STEM highlight on the following page.

LOCAL AND VIRTUAL OUTREACH

The AOEP also works with local organizations to coordinate opportunities for ARO to participate in community STEM events. These programs reach kindergarten through high school students, teachers, the general public, and other researchers through activities including career fairs, informal science activities, workshops, and seminars.

Although public health concerns surrounding the COVID-19 pandemic precluded many outreach events from occurring in person in FY21, it did provide ARO with an opportunity to participate in a number of virtual events both locally and nationwide. The following is a snapshot of the outreach opportunities that ARO participated in during FY21.

NC Science and Engineering Fair (NCSEF)

Event Description: NCSEF is an exhibition of scientific projects prepared and presented by students of all ages under the guidance of their teachers and with the help of other persons interested in the science topic. The event concludes in a competition where winners may potentially progress to compete at national and international science and engineering fairs.

NDSEG Fellowship 2nd Annual Conference

Event Description: The NDSEG conference specifically hosts Fellows in an effort to better connect them to their DoD mentors and sponsors. This information and networking event showcases DoD research as well as the research currently conducted by select Fellows.

Triangle Student Research Competition

Event Description: ARO technical PMs serve as judges for graduate-level student poster sessions, largely in the Materials Science and Electrochemistry disciplines. Judges provide feedback to the students as well as share Army research interests as it relates to their research. In addition to providing judges for the conference, a DEVCOM ARL/ARO/AEOP booth is set up to share information about Army research interests, Army S&E careers, and availability of Army graduate level scholarships and awards.

NC Masters and Ph.D. Career Fair

Event Description: DoD graduate-level scholarships and awards (Science, Mathematics, and Research for Transformation [SMART] and NDSEG) and DEVCOM ARL employment opportunities are showcased. The fair is an opportunity to gain visibility for Army research interests, collect resumes/CVs, conduct brief screening interviews, and build relationships with candidates to meet DoD hiring goals.

HSAP/URAP site visits

Event Description: The purpose of these visits is to meet with current HSAP and URAP participants to observe their daily research activities ensuring accomplishment of program objectives, introduce participants to other AEOP opportunities, showcase DoD STEM careers, and connect other AEOP participants on the same campus (virtual in 2021).
Education Outreach Program

The Scientific Services Program (SSP) was established by ARO in 1957 and is currently administered and managed for ARO through the Edmond Scientific Company (headquartered in Alexandria, Virginia). This program provides a rapid means for the Army, DoD, OSD, and other federal government agencies to acquire the scientific technical analytical 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 science and technology area of interest to the government.

The SSP awards tasks in a wide variety of technical areas, including mechanical engineering, computer sciences, life sciences, chemistry, materials science, and military personnel recruitment/retention. In FY21, five new SSP tasks were awarded with three modifications to the scope and/or funding of ongoing tasks. A summary of agencies served under this program and the corresponding number of FY21 new SSP tasks is provided in Table 1.

<table>
<thead>
<tr>
<th>Sponsoring Organization</th>
<th>SSP Tasks</th>
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<tr>
<td>DEVCOM</td>
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<td>DEVCOM ARL</td>
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<tr>
<td>Total: DEVCOM</td>
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<tr>
<td>OTHER U.S. ARMY</td>
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<tr>
<td>Combined Arms Support Command (CASCOM)</td>
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<tr>
<td>Total: Other U.S. Army</td>
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<tr>
<td>OTHER DoD</td>
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<tr>
<td>Air Force Agency for Modeling and Simulation</td>
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<tr>
<td>Joint Program Executive Office for Chemical, Biological, Radiological and Nuclear Defense</td>
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<tr>
<td>Total: Other DoD</td>
<td>2</td>
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<tr>
<td>TOTAL FY21 New SSP Tasks</td>
<td>5</td>
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</table>

Table 1: FY21 New Tasks for SSP
STEM HIGHLIGHT

Justin Jorge: Army Educational Outreach Program
Undergraduate Apprenticeship alum

To celebrate the opening of summer 2022 Undergraduate Apprenticeship applications, we spoke with apprenticeship alum Justin Jorge. Justin shares his experience with an AEOP Apprenticeship and what he’s doing now.

Tell us a little about yourself — What sparked your interest in STEM?

Since I was young, I was fascinated by how things moved. I would take apart my toys to see how the motors and springs fit together. Eventually I started repurposing parts to make my own catapults or makeshift motorboats. My interest in learning about and trying to replicate engineered systems led me to join a robotics club in high school and college. At the same time, I was also fascinated by biological motions. As a child, I enjoyed poking “rolly polly” bugs to see them curl up into balls and roll away, watching my Venus flytrap ensnare an ant, or observing other unique biological motions. I would check out books from the library to learn more about the organisms I’ve seen, or discover other biological feats. I carried my interest in biological motions with me into college where I pursued a degree in biology.

How did participating in AEOP help you in your STEM journey?

I participated in an AEOP Undergraduate Apprenticeship in 2017. Through my apprenticeship, I was given the opportunity to experience what it is like to be on the frontiers of biomechanics research. As a researcher in the lab of Dr. Sheila Patek, I used a high-speed video camera to visualize biological motions that are so fast that they are invisible to the naked eye. I found that looking at the natural world through the lens of a high-speed camera can lead to inspiring discoveries: Mantis shrimp break open snail shells by slamming them with hammer-like appendages. Snapping shrimp shoot out a jet of water from a specialized claw at such high velocities that the water around the jet boils in a phenomenon known as cavitation. Trap-jaw ants snap their large mandibles shut at accelerations similar to a bullet to capture prey or perform mandible-powered jumps by striking the ground. Looking at incredibly fast biological motions through the lens of a high-speed camera gave me the same sense of wonder as looking at a drop of pond water through a microscope for the first time.

What are you up to now?

I am currently a fourth year Ph.D. candidate in the lab of Dr. Sheila Patek. My dissertation focuses on analyzing ultrafast motions in plants – specifically plants that are able to shoot out their seeds from specialized fruits. Throughout my Ph.D. so far, I have been fortunate to share and expand my research by interacting with diverse groups. I have regularly attended SICB (Society for Integrative and Comparative Biology) to present my research to my fellow biologists in the form of talks and posters. As a part of Dr. Patek’s MURI (Multidisciplinary University Research Initiative) team I communicate with engineers, roboticists, material scientists, and other biologists to extract principles from these fast biological motions that can be used to improve man-made devices. Additionally, I presented my research at TSRC (Triangle Student Research Competition), a local poster competition that focused on material science and engineering research and was awarded with the first prize poster.

What’s the biggest lesson STEM has taught you?

The biggest lesson that STEM has taught me is the importance of community and diverse perspectives. Science is a collaborative effort and benefits from integration of the tools and minds from various fields. This is definitely the case in the field of biomechanics which lies at the interface of biology, physics, material science, and engineering. By conversing with mathematicians and physicists, I have learned about ways of analyzing my data that I would never have known. Meanwhile, the physical models made by engineers and material scientists help answer questions about biological motions that would be difficult or near impossible to test in the organism itself. Finally, when working with engineers, I enjoy sharing the wonder of a seemingly alien, biological solution to a similar design problem.
Summary of ARO Funding and Program Actions

Below is a summary of funding and program actions for FY21. The majority of the reported statistics refer only to mission-driven funds (not externally leveraged funds).

FY21 Funding Actions

PMs receive white papers throughout the year and discuss these topic ideas with the potential investigator to identify how the proposed research could better align with program vision and Army needs. Approximately one-third of the white papers received by ARO PMs from academic institutions are submitted as formal, full proposals.

White papers received in FY21
Proposals received in FY21
Total new agreements awarded following a competitive peer-review process
Agreements awarded to HBCUs/MIs
Agreements awarded through the Early Career Program

Notes: The numbers to the right refer to new-start proposals in the basic research categories: SI, STIR, ECP/YIP, HBCUs/MIs, HUB, and DURIP. Data does not include support by externally leveraged funds. Data Source: ARO New Starts in FY2021 Report.

Where ARO Funding Comes From

ARO is funded primarily from the Army and OSD. ARO funding totaled $273 million in FY21. The majority of funding that ARO receives from the Army is categorized as either 6.1 basic research or R&D basic research, and is carried in the Army’s Research, Development, Test & Evaluation (RDT&E) account. Additional sources of Army funding are provided by Congressional Additions. The amount and intended use of Congressional Additions can vary year to year. ARO is also in the unique position to leverage funds from other stakeholders including (but not limited to) DARPA, DTRA, ONR, AFOSR, USACE, and USAMRDC.


Where ARO Mission Funding Goes

ARO pursues a variety of different research programs and initiatives that have unique objectives and eligibility requirements (as described above). The ARO Core Research Program is the largest extramural funding program and is organized as a function of scientific discipline. The other ARO program and initiatives also tend to align with the Core Research Program scientific disciplines as PMs participate in topic formulation, proposal selection, and award monitoring throughout the organization.

Notes: Totals may not add due to rounding. *Congressional Additions for Basic Research are typically set aside for specific programs and/or projects. **ARO Other comprises funds set aside for ARO general and administrative support, the Minerva Research Institute, and the Board of Army RDT&E, Systems Acquisition, and Logistics (BARSL) activities. Data Source: ARO GFEBS Status of Funds Report (30 September 2023).
Core Research Program: Scientific Disciplines

How ARO Funding is Awarded

Of all of the agreements that are currently active, 83% percent of support from ARO goes to institutions of higher education. The remaining awards go to private industry, including small businesses and non-profit institutions; federal, state, and local governments; and federally funded research centers. In FY21, 508 individual organizations received support from ARO, 82 of which were designated as HBCUs/MIs.

ARO awarded funds as standard grants, cooperative agreements and contracts. Cooperative agreements are specialized grants that are used to enable substantial involvement from DoD agencies. Contracts are used to acquire products and services for DoD use, including research.

403
Total Grants

370
Awards going to U.S. institutions of higher education

82
Awards going to HBCUs/MIs

33
Awards going to International institutions of higher education

403
Total Grants

ARO’s Commitment to Capacity Building for the Nation

6,868
Total people directly supported by ARO

2,044
Faculty

904
Other Professionals

1,062
Postdoctoral Fellows

2,760
Graduate Students

98
Undergraduate and high school students

Notes: Data does not include people supported by externally-leveraged funds. Data Source: ARO Research Performance Progress Report (RPWR) Participant Counts by FY Report (12 January 2022).
Chapter 3
Success Stories

This chapter provides a brief summary of the ARO Success Stories in FY21, organized by ARO Division, Branch, and the associated Program Manager (PM) or other ARO staff. Each Success Story represents fundamental studies that will also impact one or more of the DEVCOM ARL Competencies.

This background image is from “Exploiting Ripples to Enable Layered Materials with Tunable Strength and Toughness” on page 55.
<table>
<thead>
<tr>
<th>Success Story</th>
<th>Associated ARO PM/POC</th>
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<th>SEM</th>
<th>PE&amp;QS</th>
<th>MIS</th>
<th>BBS</th>
<th>HCS</th>
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<td>Paskova</td>
<td>41</td>
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<td>Helical, Unidirectional Topological Waveguides for Integrated Photonics and</td>
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<td>Extreme Polariton Nonlinearity for Next-Generation Computing</td>
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<td>Laughing Gas Laser: Widely Tunable Compact Terahertz Gas Lasers with Nitrous</td>
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<td>ARO Investments in Self-Assembly Lead to New 3D-Printed, Multifunctional</td>
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<td>New Data-Driven Approaches for Computer-Aided Design of Soft Matter</td>
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<td>Two-Dimensional Covalent Organic Frameworks with Extraordinary Thermal</td>
<td>Varanasi, Poree, Wetzel</td>
<td>59</td>
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<td>Novel Method to Reduce Losses in Thermophotovoltaics and Other Advances in</td>
<td>Varanasi, Ulrich, Waits</td>
<td>61</td>
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<td>Emergent Matter from Assembly of Micron-Scale Atomic Origami Robots</td>
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<td>From Information Theoretic Control and Learning to Nonequilibrium Stochastic</td>
<td>Culver, Stanton, Piekarski, Spero, Garcia (retired)</td>
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Dr. David M. Stepp

Dr. Stepp came to ARO in 1999 as the Program Manager for Mechanical Behavior of Materials. He became the Chief, Materials Science Branch in 2004; the Director of Engineering Sciences in 2016, and the ARO Chief Scientist in 2020.

Dr. Stepp completed his undergraduate studies at Harvey Mudd College, receiving his B.S. in Engineering in 1993. He studied Mechanical Engineering and Materials Science at Duke University, receiving his Ph.D. in 1998.

Scientific Discovery and the Army: Science ≠ Technology

Across the Army, and DoD, the term “science and technology (S&T)” is used as a general description or category of scientific discovery and technology development efforts. While this broad categorization is appropriate for distinguishing, for example, S&T from acquisition, it can also lead to a gross misunderstanding of the inherent distinctions and relationship between science and technology. This oversimplification poses a tremendous threat to the Army’s efforts to operationalize science and equip the future Soldier.

Science seeks to discover the laws that govern the known universe and the relationships between them. It is a methodical and iterative process. By employing the scientific method—forming testable explanations, making predictions, and testing those predictions—knowledge is continually built, refined, and organized. Perhaps Henri Poincaré put it best, “The aim of science is not things themselves...but the relations between things.

Technology seeks to apply these scientific laws and relationships, and sublimate them into devices and products. Technology focuses on the techniques, skills, methods, and processes necessary to produce goods and services, or accomplish specific objectives. The aim of technology is the implementation of knowledge.

When science is misunderstood or oversimplified as technology, the “things” become the aim, and scientific discovery is deprioritized or abandoned for technology development. The Army has an acute awareness of its need for new technology, and disruptive scientific discoveries offer unprecedented opportunities for transformational overmatch; therefore, decisions to support technology transitions over scientific discovery are often easily rationalized by Army leaders in support of their mission.

To complicate matters further, the return on investment of scientific discovery is nearly impossible to calculate precisely but frequently grows exponentially over time. As a result, the costs and risks associated with redirecting resources from scientific discovery to technology development are ill defined and often underestimated. Decreasing support for scientific discovery threatens the Army’s efforts to operationalize science, both in terms of a failure to discover new knowledge (i.e., especially when scientific discoveries cluster in new areas and between traditional scientific disciplines) and in terms of a failure to consume that knowledge for the Army (i.e., talent management). Similarly, excessive investment in immature technology often leads to flawed estimates of its future value. Chemical and Engineering News captured a particularly Army-relevant example of this on its June 8, 2015 cover, titled, “What Happened? We Were Promised a Carbon Nanotube Revolution” (reflecting on 15 years of expectant investment in carbon nanotube research predicting $100M markets that still have not been realized).

Operationalizing science cannot succeed merely by enhancing or accelerating technology transition. History shows us such approaches often miss the robust integration required to exploit a new scientific discovery for revolutionary technology. To succeed, the Army must do the difficult and relationship-centric work of integrating scientific discovery with technology development through partnerships that establish lasting collaborations and provide opportunities for cyclic iteration between the two. Science provides and refines knowledge, and there is great opportunity at the boundaries of dissimilar fields and bodies of
knowledge. Insights here are neither trivial nor easily obtained, but can have profound ramifications for technology development. Furthermore, the relationships between scientific discovery and technology development mature and grow more robust with time and study. Operationalizing science requires the establishment of deep and enduring relationships across the science and the technology enterprises that allows for questioning, feedback, testing, and assessment across both domains to facilitate the agile and heavily interdependent advancement together. We must build a network, not a pipeline.

What’s more, integrating Army-centric S&T requires rich collaboration with the Warfighter to assure the right science is considered and the right products are developed. Thankfully, we are now building collaborations between AFC DEVCOM scientists and AFC Futures and Concepts Center concept developers at the working level. Scientists and technologists across the Army alike have been introduced to the Army Functional Concepts (i.e., the capabilities the Army expects to have 6 to 18 years in the future), the Army’s process for concept development, and how Army concepts connect to Army requirements and systems acquisition. It should not be surprising that the first conceptor–scientist workshop was hosted by ARO in 2020. Of course, such collaborations require careful attention to the distinctions between scientific discovery and technology development. With this in mind, a guiding analogy has emerged: scientific discovery is to Army concepts as technology development is to Army requirements. As technology development must both be responsive to and drive Army requirements, scientific discovery must be responsive to and drive Army concepts. Furthermore, attempting to connect scientific discovery directly to Army requirements (or technology development directly to Army concepts) most often leads to technology transition failures. For a full discussion of the recommended Army concept-centric process tenants, see “Proposed Army Futures Command Process Tenets”.

Finally, it is important to note that science and technology do not easily form a single, balanced, or self-propagating community or enterprise for the Army. There is a constant tension between new scientific discoveries, which shape and refine how we understand the universe, and the development of things, which shape and manipulate that same universe. Scientific discovery is often interpreted as independent from Army operational guidance or needs, consuming resources that would be better directed toward specific objectives. Similarly, technology development is often seen as lacking a robust scientific foundation, being incremental, and being of questionable cost-effectiveness. Nevertheless, this tension brings the opportunity for extraordinary breakthroughs in both disciplines. By forming lasting partnerships that allow feedback, ongoing bidirectional communication, and iterations between science and technology, the enterprise becomes greater than the sum of its parts. Scientific discoveries (and failures) can become the foundation for new paradigms of technology. Technology development breakthroughs (and barriers) can provide new perspectives to inspire the discovery of even more extraordinary science. The fields of electronics, advanced materials, artificial intelligence, cybersecurity, and synthetic biology are full of such examples; scientists and technology developers (including broad industry partners) built lasting relationships that drove unprecedented advances. The premier example of this is Bell Labs, which is credited with developing dozens of new technologies and nine Nobel Prizes. Another noteworthy example is SEMATECH, the consortium formed by 14 major American semiconductor manufacturers and the U.S. government that brought the country’s semiconductor industry from the edge of collapse to the world leader in less than 10 years. This was accomplished by focusing on improving manufacturing competence (i.e., developing new techniques and equipment) rather than end products.

Rather than a linear pipeline of simple and harmonious development, science and technology seem to come together more effectively as countercurrent exchange. The “flow” of scientific discovery and technology development are not parallel; they are different and can face unique challenges (i.e., discovering a new material property and manufacturing that material in bulk). Similarly, the crossover and interchange between the two usually occurs orthogonally to either flow. What is considered most significant in one is not the primary focus of the other, and may even be viewed as trivial. This is why it is essential to forge a community based on respect and trust. A successful integration of the S&T enterprises requires lasting partnerships where the richness of each contribution can be cultivated and manifested successfully in the other discipline. Again, we must build a network, not a pipeline.

The ARO Year in Review captures an extraordinary set of examples where scientific discovery has created astonishing turning points for humanity, altering our understanding and enhancing our ability predict the universe and its interactions. They articulate diverse efforts over a range of maturity levels, each having a different and unique impact on Army technology. However, no discovery simply “becomes” technology without considerable interchange, translation, and partnership among scientists and technology experts. Rather, extraordinary scientific discoveries, like those captured in this document, inform decisions on opportunities to build game-changing future technology programs for the Army. They provide initiation points and break current barriers for operationalizing science with disruptive new scientific paradigms that, when brought into a network of collaborations and lasting partnership, inspire and inform opportunities for new technology development efforts to provide the future Army operational overmatch.
BIOTRONICS PROGRAM

Program Manager
Dr. Albena Ivanisevic

Dr. Ivanisevic completed her undergraduate studies at Drake University, receiving her B.S. in Chemistry in 1996. She trained as a surface chemist at the University of Wisconsin–Madison, receiving her Ph.D. in Inorganic Chemistry in 2000.

She came to ARO in 2020 as the Program Manager for Biotronics after 18 years as a faculty member at Purdue University and North Carolina State University.

Current Scientific Objectives

1. Achieve control of useful material systems that can be used to influence and probe cells via their bioelectronics-dependent behavior that, if successful, will enable future read-outs and actuation technologies to interrogate cellular activity, which could lead to future body-heat–powered devices to modernize Soldier lethality and biocompatible electronics to augment Soldier performance.

2. Probe living cells’ intrinsic bioelectric fields from the “outside” (no cell penetration) using electronic modalities that, if successful, will enable novel electrochemical sensors to track key biomarkers, which could lead to wearable body sensors and control systems for expeditionary Soldier and environmental sensors with high sensitivity and survivability in harsh conditions so Soldiers can quickly understand and react to emerging situations, thus increasing their lethality, precision, and survivability.

SUCCESS STORY

Critical Phenomena in a Nanoparticle Necklace Network: A New Principle for Metallic Transistors

ARO-initiated research has resulted in the development of a new principle to make a transistor from 10-nm gold (Au) particles. The transistor operates at room temperature with 10³-fold higher gain than today’s metal devices, which require cryogenic temperatures. The new principle is based on hierarchical field-activated tunneling of electrons (FATE).

CHALLENGE

In principle, all-metal transistors with nanostructured interfaces have the advantage to directly couple with the membrane potential of thick-cell-walled microorganisms to enable gating—a “living biotransistor.” The biotransistor is an ideal “voltmeter” to measure the biochemical activity of cells in real time and develop highly specialized devices using bioengineered microorganisms. The challenge is that the gating effect (the ability to turn the transistor on and off) vanishes at temperatures relevant for bioactivity: on the order of room temperature. A novel architecture of metal nanoparticles has been found to exhibit a conduction gap at room temperature, and as such, it is a promising design to develop all-metal biotransistors. The architecture, called a nanoparticle necklace network (N³), is a random network of strings (or necklaces) of nanoparticles. Although N³s exhibit identical characteristics to the well-known, all-metal Coulomb blockade devices operating at cryogenic temperature, theoretically this gating effect should vanish at room temperature. A new device physics principle is needed to leverage the non-ohmic behavior (that is, switching behavior) of N³s to develop a high-gain, all-metal transistor.

ACTION

Dr. Ivanisevic initiated a discussion with Professor Ravi Saraf from University of Nebraska–Lincoln to leverage the unique electrical behavior of N³s to seek an approach to achieve gating with high gain and then couple it to microorganisms. Leveraging the network-like geometry of N³, Professor...
Saraf proposed performing rigorous analysis of the structure to understand the anomalous electronic behavior, which may lead to a strategy to make a high-gain transistor to interface with microorganisms. The discussions resulted in Dr. Ivanisevic funding an exploratory grant to develop and study an all-metal living transistor in 2021.

**RESULT**

The key innovation is the special architecture of the device channel—the N3 (Figure 1). One-dimensional necklaces of 10-nm Au particles are made by directed self-assembly. The necklaces are deposited by centrifuge to form a self-limited monolayer to form a 2D network. The N3 exhibits a robust single-electron effect (i.e., Coulomb blockade) at room temperature using large particles (~10-nm diameter). Usually, to obtain a Coulomb blockade at room temperature, the particles are <3 nm, which have significant quantum noise due to their sensitivity to size caused by thermal expansion. The networks’ structural complexity makes the transistor about 1,000 times more responsive to external stimuli than today’s most advanced metal devices (Figure 2). The study marks the first time an Au necklace structure has been used in a transistor, and the approach is enabling Professor Saraf’s team to overcome the longstanding obstacle of the Coulomb blockade effect. The necklace-like morphology circumvents that problem by introducing a complex network that dictates the channels through which current can pass. Professor Saraf analogizes the setup to the thousands of interstates, highways, streets, and dirt roads that connect the East and West Coasts of the United States. Under the conventional Coulomb blockade approach, the “traffic flow,” or current, is regulated by putting up small barricades, in the form of a single electron charge, across most major thoroughfares. But at room temperature, the barriers are overcome, erasing the effect. In contrast, the N3 is akin to opening more roads for traffic offering similar transport and regulation capabilities as a Coulomb blockade at higher temperatures. The room-temperature performance is the key advance needed for further development in bioelectronics, as cryogenic temperatures would inhibit biological activity.

**WAY AHEAD**

The next goal is to develop an array of “living biotransistors” gated by individual cells in a microbe colony. The success will establish a platform to study the emergence of antibiotic resistance. By concomitantly recording individual cells in a colony, new insight on cell-cell communication in real time can be gained with applications in synthetic biology, quorum sensing, and spatial heterogeneity of persister/nonpersister states.
SUCCESS STORY
Self-Sustaining, Intelligent Microsystem Made from Green Biomaterial

A microsystem emulating both the signal processing and material composition in a biosystem is constructed to show intelligent autonomy (Fu et al., 2021). Continuous development may lead to future self-sustaining intelligent systems in various environments.

CHALLENGE

Biological life features autonomy with intelligent response to environments, owing to the high efficiency in signal retrieval and processing. Lifeforms use a common signal of an ultra-low amplitude (e.g., 10 times lower than that in electronics) to save energy for improved sustainability. Also, the signal is processed and stored at a local unit (e.g., a neuron) to save data traffic. These strategies enable an efficient detection-decision-action cycle. For example, a signal retrieved from the sensory organelle can be readily processed by the neuron for a decision, saving both the time and energy involved in signal “translation” that is usually involved in current electronic systems. Therefore, emulating signal processing with a matched amplitude to biosystems is key to developing systems of high-level autonomy and intelligence.

ACTION

To address this challenge, Dr. Ivanisevic initiated a discussion with Professor Jun Yao from the University of Massachusetts Amherst, whose team has been developing novel electronic devices by “borrowing” both material and functional principles from biosystems. Professor Yao has harvested protein nanowires from the microbe Geobacter sulfurreducens (Lovley et al., 2021) (Figure 3). These nanowires are conductive and an exciting biomaterial, which are used to construct the key components in a microsystem (Fu et al., 2021). Specifically, the protein nanowires are used to create an artificial neuron that can mimic signal processing in a neuron. Importantly, the protein nanowires confer a unique catalytic effect, which enables the artificial neuron to work with signals matched to biological amplitudes (e.g., <0.1 V) (Fu et al., 2020). Electronics constructed from the artificial neuron can then directly process environmental signals without the need for translation (e.g., amplification) to standard electronics. Meanwhile, the protein nanowires can be also used to make thin-film devices (termed “air-gen”), which can harvest electricity from the ambient humidity (Liu et al. 2020). Based on these discussions Dr. Ivanisevic funded Professor Yao to study fabrication of devices that contain a pair of interdigitated electrodes.

“We have demonstrated fully self-sustained neuromorphic interfaces, which are based on a marriage between bio-amplitude signal processing and ubiquitous environmental energy harvesting, both enabled by the unique properties in protein nanowires. This marriage leads to comprehensive functionalities that are advantageous to those in existing neuromorphic interfaces. It also fundamentally closes the gap to biological integration that features a high level of intelligent signal processing and energy self-sustainability.”

– Fu et al. (2021)

RESULT

Protein nanowire films were deposited on the bottom electrode and covered by the top electrode. The devices were sealed between two layers of polymer film to maintain the mechanical integrity and at the same time permit exposure of the protein nanowire films to ambient humidity. The devices were utilized in a series of proof-of-concept studies (Fu et al., 2021). In one of them, Professor Yao’s team showed that the vertical protein nanowire device can serve as a continuous energy source to drive other sensory interfaces. The interfaces responded to different stimuli, transcending specific-stimulus-typed interfaces relying on the careful selection of sensors to achieve a signal match to memristors. When a passive pressure sensor was combined with the protein nanowire device to form an active tactile receptor, the resistance change in the pressure sensor was converted to an active voltage signal. This led to charging in the membrane potential
and subsequent neuronal firing. In a similar manner, replacing the pressure sensor with a passive optical sensor yielded an afferent optical neural interface. Optical stimulations were converted to active voltage signals that could drive the neuronal firing. These results demonstrate the versatility in achieving self-sustained, multifunctional neuromorphic interfaces that can perceive and process different stimuli. These interfaces, which are fully environmentally driven, are inherently different from previous systems that either required external powering or were restricted to a specific type of stimulus for the signal match to memristors. The team points to two factors responsible for the difference: (1) humidity is ubiquitous and hence provides truly continuous powering and (2) the bio-amplitude signal processing removes the fundamental barrier in a signal mismatch. This first-of-its-kind biohybrid electronic device demonstrated the capability to harvest energy from humidity while simultaneously electrically responding to multiple types of external stimuli.

WAY AHEAD

The research points to a more-intimate common ground between electronics and biosystems. As a result, it can enable the feasibility of constructing advanced bioelectronic interfaces, in which electronics may directly “talk” to biosystems, transcending current ones involving various indirect signal “translation.” Therefore, the research team will next attempt to develop biosensors that can retrieve a signal from biosystems and investigate the possibility of using the signal to directly drive the electronics for computation. If successful, the research is expected to advance the intimacy in bioelectronic interfaces, which will eventually contribute to advanced human technologies in, for example, prosthetics and performance augmentation. It is also expected to support development in hybrid bio-bots and living microsystems.

**Results**

- Fabricated a self-sustained intelligent microsystem.
- Demonstrated the use of artificial neurons in computation—it is particularly exciting that the protein nanowire memristors show stability in aqueous environment and are amenable to further functionalization.
- Determined that additional functionalization not only promises to increase microsystems’ stability but also expands their utility for sensor and novel communication modalities of importance to the Army.

**Anticipated Impact**

The work contributes to knowledge of integrating bio-inspired microsystems. The prototype emulates biological signal processing to realize intelligent autonomy like a living organism. The research and future research could lead to intelligent systems with self-sustainability deployed in various environments and enhance the Army’s Modernization Priority that supports Next Generation Combat Vehicles.
Dr. Tania Paskova obtained her M.S. in Microelectronics in 1984 and Ph.D. in Physics in 1993 from Sofia University, Bulgaria. She trained as a physicist and crystal grower at Linkoping University, Sweden.

She came to ARO in 2020 as the Program Manager for the Electronic Sensing Program after more than 25 years’ experience in academia, industry, and government.

SUCCESS STORY

Nanostructured Black Phosphorous and Meta-Structure Integrated Absorbers for Efficient Light Trapping in the Mid-Infrared Region

This Army-funded research has developed new methods for nanostructuring and integrating innovative metastructure absorbers with efficient light trapping in the mid-wavelength IR (MWIR) region. Such engineered heterostructures with enhanced absorption polarization sensitivity will enable advanced IR photodetectors with designation capabilities allowing superior detection and situational awareness.

CHALLENGE

Modern photodetectors operating in the MWIR band of the electromagnetic spectrum require cooling well below 180 K to achieve high detectivity while minimizing the undesired dark current. An effective MWIR detector usually uses a thicker absorber layer, on the order of cutoff detection wavelength, to enable high quantum efficiency, flatter bands for suppressing undesired Auger generation and recombination, and low defect density for longer Shockley–Read–Hall lifetimes. These characteristics are very challenging to simultaneously achieve at elevated temperatures. In recent years, various approaches have been proposed to increase the operation temperature, including photon trapping, plasmonic structures–coupled detector designs, advanced barrier architectures including superlattice (SL) elements, etc., but the improvements are still limited to 200 K, well below room temperature (RT). For example, the most established mercury cadmium telluride (HgCdTe) MWIR detectors are now operating at or below 160 K, and Type-II SL detectors typically operate at or below 150 K.

ACTION

To facilitate addressing these long-standing challenges, Dr. Michael Gerhold and Dr. Paskova have looked at alternative material platforms and device concepts with novel functionalities that could fulfill the harsh requirements for RT detection with high sensitivity. Among various options, MWIR detectors based on the emerging low-dimensional—2D and quasi-1D—materials attracted the researchers’ interests due to their unique characteristics differing from their bulk counterparts. Dr. Gerhold dug deeper and

This success was made possible by:

Drs. Michael Gerhold and Tania Paskova, Electronics Branch

Citations:


sought information in many forums from Defense Advanced Research Projects Agency (DARPA) program reviews to Joint Technology Office meetings, and he recognized that the 2D materials integrated with possible metamaterials (engineered to have properties that are not found in naturally occurring materials) could provide a new technology base for advanced IR photodetectors with exceptional performance. In 2018 he funded a new Single Investigator (SI) project led by Professors Han Wang and Michelle Povinelli at the University of Southern California to both experimentally and theoretically explore such novel platforms.

Similarly intrigued by novel engineered material systems, Dr. Paskova in 2017 gave a keynote talk at SPIE Optics + Photonics, San Diego, focused on emerging electronic and photonic materials and engaged in multiple conversations on metamaterials’ unique properties and potential. What emerged was the incredible flexibility to manipulate the properties of these structures in very wide ranges. This indicated the strong need for theoretical simulations targeting designs and predicting precise characteristics for specific applications in order to guide the experimental efforts. The collaborative project by Professors Wang and Povinelli benefits from such complementary theory/experimental thrusts, and Dr. Paskova continues to support this team effort as well as other research teams exploring integrated metasurfaces for MWIR applications.

**RESULT**

The family of 2D and layered materials has been rapidly expanding, but within this large variety of hundreds of materials, black phosphorus (BP) and its isoelectronic group IV monochalcogenides have a unique place. These puckered materials have distinctive crystalline symmetries and exhibit exciting properties, such as high carrier mobility at RT, strong responsivity, widely tunable bandgap (achieved by controlling the layer number and external fields), in-plane anisotropy, and spontaneous electric polarization.

Professors Wang and Povinelli focused their initial efforts on developing a new method for large-area BP thin film synthesis, which included two steps: (1) physical vapor deposition of a red phosphorus (RP) thin film at 400 °C, followed by (2) high-pressure high-temperature conversion of RP into BP, the most stable allotrope of phosphorus. Having such large-scale, high-quality materials available allowed a thorough evaluation and in-depth understanding of the carrier transport in BP and demonstration of a BP detector with room-temperature detectivity above $9 \times 10^9$ Jones even without enhancement. The team also developed a metasurface model and then designed and fabricated integrated light-trapping structures (Figure 1) that are essential for optimizing BP thin films to absorb light in the MWIR spectral range.

In early 2020, the research team experimentally validated their theoretical simulation, indicating a significant enhancement factor due to the metal-insulator-metal (MIM) device (Figure 2a) integration. The researchers conducted an experiment with a gold nanostructured design in thin BP films to determine the absorption in the 3–5 μm wavelength range. By suitably tuning the design parameters of the MIM structure (Figure 2b), lateral resonance modes can be excited in the BP layer. They compared the absorption enhancement due to the resonant light trapping effect to previously reported improvements with alternative methods. For a layer thickness of 5 nm, an enhancement factor of 561 was achieved at a wavelength of 4 μm, significantly greater than the anticipated conventional limit. The ability to achieve strong absorption enhancement (Figure 2c) in ultrathin dielectric layers, coupled with the unique optoelectronic properties of BP, makes this absorber design a particularly promising candidate for MWIR photodetector applications.

In their most recent effort, the researchers paid special attention to exploring the detection of polarized light as a tool that can enable a multitude of new functionalities in photodetectors, such as extraction of the 3D geometry of an object, high-accuracy sensing under very weak light signals, and a significantly enhanced sensing range in dusty and foggy conditions. In addition, the ability to dynamically tune the bandgap of BP...

**Anticipated Impact**

The research is expected to provide a better understanding of emerging MWIR material and device innovation through integration with metastructures, enabling high-performance RT MWIR detectors that can potentially benefit many Army sensing and imaging applications.

**Results**

- Displayed a new synthesis method for achieving large-scale BP thin films.
- Demonstrated a high-performance MWIR BP detector operating at RT.
- Integrated MIM gratings with BP photodetector structures to increase light absorbed by the BP film.
- Led to publications in Nature Review Physics, Optics Express, and Nano Research.
thin films through applying a vertical electrical field can turn each pixel into a spectrometer and lead to novel hyperspectral sensing capabilities such as programmable on-chip mid-IR spectroscopy.

The program involves collaborations with DEVCOM ARL, including the exchange of ideas, data, and samples. Particularly important is the discussion on optoelectronics research with Dr. Matthew Chin, a researcher at DEVCOM ARL’s Sensors and Electron Devices Directorate.

WAY AHEAD

Professors Wang and Povinelli will work to further improve the material synthesis, to explore vertical vs. lateral BP detector designs with various types of integrated metastructures, and to confirm their theoretical predictions. For example, their predictions suggest more than 100 times greater absorption, RT detectivity greater than $5 \times 10^{11}$ Jones (surpassing the $10^{10}$ Jones in current state of the art) with enhanced polarization sensitivity and wider detection angle. A successful validation is expected to lead to an ambitious goal—namely, to prove that metastructure integration is a powerful concept for color sensitive single photon detection in the MWIR.

SUCCESS STORY

Stacking and Twisting van der Waals Heterostructures for Ultrafast, Ultrasensitive Vibronic Sensors

This ARO-funded research leverages a newly discovered property of ultrathin van der Waals (vdW) semiconductors—molecular-like vibronics (coupled vibration and electron) within a solid-state semiconductor device—to enhance the energy transport toward the quantum limits in efficiency. The explored p-n junction photodiodes are designed to exploit this capability to emit and absorb at IR wavelengths and potentially operate at terahertz speeds. If successful, this approach will spawn a new generation of truly quantum photodiodes that operate at RT, a sought-after operational element for quantum communication networks, next-generation photovoltaics, and ultrasensitive single photon sensors.

CHALLENGE

Two-dimensional vdW heterostructures are materials made up of layers of single-atom-thick sheets like a stack of paper and in which the atoms are strongly bonded in the sheet and weakly bonded between the sheets (Figure 3). When two vdW materials are stacked together, the lattice mismatch and/or twist angle between them can generate a nanoscale moiré pattern, which sporadically modulates the interlayer interaction and forms periodically distributed moiré potential wells. The resultant moiré superlattices can exhibit strong correlation effects, including insulating, superconducting, and magnetic phases. With respect to optical properties, semiconductor moiré superlattices can confine excitons (electron-hole pairs held together by the electrostatic Coulomb force) in the moiré potential wells with distinctive properties that can be used to realize artificial excitonic crystals as a novel quantum platform. However, a deep understanding of how excitons interact with other carriers is needed to exploit their full potential and have full control of and the ability to manipulate their properties for desired purposes.

ACTION

During Dr. Paskova’s tenure at the National Science Foundation as a Program Director for the Electronic and Photonic Materials program, several innovative proposals caught her attention, focusing on novel methodologies to engineer artificially stacked 2D vdW materials. These materials are expected to have unprecedented properties along with advantages such as scalability, enormous choice of compositions, and access to properties, functionality, and behavior that does not exist in nature. One of these proposals was submitted by Professor Nathaniel Gabor (University of California, Riverside) and was selected for a CAREER award. Shortly thereafter, his group reported new discoveries of a giant intrinsic photoresponse in pristine graphene (Nature Nanotechnology, 2019) and an electron-hole liquid in a vdW heterostructure (Nature Photonics, 2019). While monitoring the topic closely, Dr. Paskova was drawn to another publication by this team, reporting on the
enhancement of fast and sensitive IR light sensing in prototype quantum sensors based on stacked and twisted quantum materials (Nature Nanotechnology, 2018). Dr. Paskova recognized the potential of this novel approach and had in-depth discussions with Professor Gabor’s team about their observation of extremely strong exciton-vibrational coupling when individual vdW layers are combined to form atomically thin heterostructures. IR photoresponse of interlayer excitons showed features of molecular-like vibronic physics, the key requisite for quantum coherence in the electron-hole pair separation process and their potential for quantum 2D p-n junction photodetectors. Following-up, she encouraged a proposal submission and funded an SI grant with the goal of exploring the ability to stack-engineer 2D material platforms that could enable the interaction between vibrational motion and electronic states—a novel hybrid concept that, if successful, will herald a new era of quantum sensor science.

RESULT

The effort started by exploring the optical properties of tungsten diselenide (WSe2)/ tungsten disulfide (WS2) heterobilayers formed by stacking WSe2 and WS2 monolayers. By introducing an interlayer rotation angle, the heterostructure can be tuned at nanoscale; a 60° interlayer rotation yields a moiré pattern with a period of ~8 nm. Within such a pattern, an electron (hole) density of ~1.8 × 10¹² cm⁻² can fill one angle, the heterostructure can be tuned at nanoscale; a 60° interlayer rotation yields a moiré pattern hybrid concept that, if successful, will herald a new era of quantum sensor science.

Moreover, by finely controlling the spacing of moiré trions, which can be tuned by the relative twist of the individual layers, the team has laid the foundation for a new class of exciton quantum devices that go beyond the current capabilities achieved in nanofabricated quantum dot arrays.

Beyond the discovery of a new type of trion, the team then identified extraordinarily strong exciton-phonon coupling in the optoelectronic response of WSe2/molybdenum diselenide (MoSe2) heterojunction photodiodes. To access the vibronic physics of this system, which is most commonly observed only in molecules, the team introduced photocurrent spectroscopy. Using precisely designed optoelectronic devices, photocurrent spectroscopy serves as a sensitive technique for probing interlayer excitons, which are difficult to observe via reflectance contrast and photoluminescence (PL), the absorption and emission properties of the superlattice were revealed, showing significant interlayer exciton PL even at RT, indicative of high device quality. Remarkably, the WSe2 moiré excitons were found to exhibit spectral modulation at fractional fillings (ν = 1/3, 2/3) in the WSe2/WS2 moiré superlattice. Such significant modulations of absorption, emission, and valley polarization of excitonic states in a moiré superlattice indicate an unprecedented level of direct access to the superlattice properties using optical and optoelectronic techniques.

Furthermore, the team reported moiré trions (a localized excitation that consists of three charged particles coupled to the moiré superlattice potential). These interlayer moiré trions combine both the properties of excitons (such as sharp optical resonances and strong quantum confinement) and electrons (localized electronic charge and electrical control). In sharp contrast to conventional trions that are not confined to specific locations within a crystal, interlayer moiré trions are highly confined to a regular spatial pattern with only a few nanometers between each trion throughout the entire crystal. These findings could have important implications for future technologies, since the periodic array of moiré trions acts as an ultra-high-quality array of quantum dots that can be electrically controlled and optically addressed. Moreover, by finely controlling the spacing of moiré trions, which can be tuned by the relative twist of the individual layers, the team has laid the foundation for a new class of exciton quantum devices that go beyond the current capabilities achieved in nanofabrikated quantum dot arrays.

Way Ahead

This research is among the first to explore the ability to stack-engineer the interaction between vibrational motion and electronic states, potentially opening a new direction for quantum sensor science and technology. The results represent foundational steps in vdW structure design that could lead to a new generation of vibronic devices, operating at RT for applications in quantum communication and quantum sensors in support of the Army Modernization Priority of Network C3I. The early accomplishments have already generated substantial interest both within academia and beyond. As the research continues, Dr. Paskova will continue to capitalize on opportunities to connect Army and DoD researchers to this research area in order to accelerate the identification of new technology and innovations that could enable superior sensing and communication capabilities.

ARO Competencies:

Photonics, Electronics, and Quantum Sciences

Electromagnetic Spectrum Sciences

Results

• Demonstrated evidence for a new type of quantum excitation (i.e., interlayer moiré trions in vdW heterostructures).

• Revealed vibronic exciton-phonon states in the interlayer quantum transport of interlayer excitons.


Anticipated Impact

The research is expected to contribute to a better understanding of novel optoelectronic properties in stacked and twisted 2D quantum materials and high-performance devices involving the physics of quantum processes in light sensing that could lead to the development of ultrafast, ultrasensitive vibronic sensors and other electronic devices.
SUCCESS STORY
Helical, Unidirectional Topological Waveguides for Integrated Photonics and Polaritonics

Topological physics designs in the areas of nanophotonics and nanoscale modulators resulted in unidirectional propagation that can have a transformational impact on integrated photonics. Particular advances are likely in areal density of photonic devices and optical isolation of devices for increased performance and reliability.

CHALLENGE
The ability to efficiently modulate light at the nanoscale and transport the information over long distances with very low loss is a major challenge in nanophotonics. Overcoming these challenges can be tremendously beneficial for developing the next generation of integrated photonics infrastructure. Future optoelectronic devices must deliver significant improvements with respect to size, speed, and power efficiency. Typically, on-chip silicon-based optical modulators require a large device area to manipulate light because of the very weak light–matter interaction strength of the material. In addition, transport of information across conventional waveguides is lossy; scattering and back-reflections lead to significant power loss and require isolators that result in further power losses. In addition, conventional waveguides need to utilize a larger area to bend light due to diffractive losses, limiting the bend radius to more than a few times the optical wavelength. Therefore, new materials and innovative device architectures are required to modulate light at the nanoscale and route the information in optical waveguides that can bend at arbitrarily small radii with minimal scattering and back-reflection losses. Research based on ideas from topological physics applied to optics combined with the extremely large light–matter interaction strengths of 2D materials can help solve many of these very challenging technical limitations that may not have solutions in more conventional approaches.

ACTION
Dr. Gerhold began interacting with Professor Ritesh Agarwal at the University of Pennsylvania in 2013 after inviting him to speak at the IEEE Photonics topical meeting on nanowire photonics. ARO’s Electronics Branch was already familiar with Professor Agarwal’s work; he spoke at their 2011 Electronics Strategy Planning Meeting on related topics. Subsequent discussions and formulation of
ideas led Dr. Gerhold to award a collaborative agreement to Professor Agarwal and Professor Volker Sorger of The George Washington University in 2016 on the topic of energy-efficient nanoscale modulators based on 2D materials. The grant award titled “2D Material based Electro-Optic Modulation on a Silicon Platform” was to explore a path for nanoscale, attojoule per bit efficient, ultrafast electro-optic modulators where the index of refraction of 2D materials can be actively altered. To accelerate the work, an instrumentation proposal was also awarded for a magneto-optical cryostat so that low-temperature phenomena could be investigated. The efforts were highly successful, resulting in the demonstration of novel electro-optic modulators utilizing a variety of promising 2D materials that can be integrated with conventional silicon platforms.

RESULT

Topological physics, including extensions to photonics, is very promising for finding new solutions to problems in electronics and optoelectronics that can lead to energy-efficient devices immune to power loss from defects and disorder. For example, Professor Agarwal demonstrated the first “helical topological polaritons,” a new, promising combination of robustness from topology with 2D materials (Figure 1). This approach can be very attractive for assembling nanoscale modulators integrated with topological waveguides. Owing to the increasing appreciation of the role of topology in both electronic and photonic systems, polaritons, which are half-light–half-matter quasiparticles resulting from the strong hybridization between excitons and photons, are an important platform for building actively controlled topological devices. Unlike photons, topological polaritons can be actively manipulated via external fields and are promising for actively controllable topological devices. Thus, they inherit useful properties of both photons (fast operation speed, and large spatial and temporal coherence) and excitons (large nonlinear susceptibility and electric-field control).

A previous breakthrough demonstration of topological polaritons was at 4 K and required very strong magnetic fields to induce the topological nature into the polaritons. This is not compatible with integrated photonics. Therefore, the challenge Professor Agarwal faced was to design a new system that could lead to a topological phase of polaritons but at higher temperatures and not requiring external magnetic fields. Professor Agarwal and his team came up with an innovative design by combining the unique properties of excitons in 2D materials with an underlying helical topological photonic lattice cavity. This cavity was exquisitely designed to strongly couple photons with 2D excitons and hence form a new phase of helical topological polaritons. This phase is stable up to 200 K, a great improvement over previous approaches. The unique helical nature of the topological polaritons was experimentally verified where polaritons corresponding to the opposite helicities were transported in opposite directions negotiating very sharp bends along the topological waveguide interface with no observable backscattering (Figure 2). Very small changes in external stimuli, such as temperature, electric field, or strain, were shown to induce dramatic changes in the polariton properties while preserving their

Anticipated Impact

Integrated photonics implications for the Army include faster processing performance due to increased device density made possible by reduced bending radius and increased isolation between devices.
This success was made possible by:

Drs. Mike Gerhold and Marc Ulrich, Electronics Branch

Citations:


topological robustness. This breakthrough demonstration paves the way for fabricating compact, tunable polaritonic devices for robust classical and quantum information processing applications (Figures 3 and 4). The results were published in the journal Science in October 2020.

WAY AHEAD

The next steps are to explore the applications of topological waveguides and modulators for integrated photonics for compact and robust performance leading to significant improvements in device and photonic circuit metrics. The goal of future work will be to establish solid evidence of how the approaches can be used in large-scale nanofabrication foundry processes. In particular, a demonstration of the novel topological waveguides within a state-of-the-art 45-nm node photonic circuit manufacturing process would enable DoD and industrial photonic integrated circuit designers to incorporate the functionality into optical signal processing technologies. The outcome could be significant miniaturization and optical isolation afforded by Professor Agarwal’s unique waveguides.

SUCCESS STORY

Extreme Polariton Nonlinearity for Next-Generation Computing

ARO-funded researchers at the City College of New York (CUNY) have demonstrated strong light–matter interactions in 2D materials within microcavities (known as “exciton-polaritons”) with nonlinearities that should enable powerful computing regimes.

CHALLENGE

Photonic computing presents an outstanding opportunity for higher-performance (operations/second and energy efficiency) operations. Photons, unlike electrons, can occupy the same space at the same time. However, the limitation in achieving a true optical computing regime has been in achieving a low-energy switching operation that can change the state of the system and solve a mathematical problem. Polaritons—specifically, exciton-polaritons—enable such state switching by creating a state that couples light (a photon) to matter. In this case, the matter is an electron-hole pair known as an exciton. Two-dimensional materials elevate this pursuit by providing a strong excitonic state that maintains its viability at room temperature or above. Prior research in this regime with semiconductors such as gallium arsenide (GaAs) was limited to cryogenic temperatures. The challenge has been to harness the polaritons such that they can be used for computing. Such regimes are thought to hold great potential impact on computing due to the extremely low threshold energies needed to create condensates of polaritons—that is, where all the polaritons are in a single coherent state. The coherence of such polaritons at room temperature has been shown to occur at 3 to 4 orders of magnitude lower photon intensities than photon lasers. Coherence provides a means for spatial interference within the condensate that can be used for computing. Achieving the polaritonic condensate and using it in a computational paradigm has been a challenging materials, physics, and optoelectronic engineering problem.

ACTION

Dr. Gerhold began investing in the field of polaritonics over a decade ago, including Professor Vinod Menon’s work at CUNY. In those early years, Professor Menon wrote an editorial to Nature Photonics in 2010 explaining how room-temperature polaritonics may provide a future to low-energy optical computing and signal processing (Menon et al., 2010). Professor Menon’s subsequent award to utilize nanostructured materials in optical cavities for enhanced polaritonic features culminated in recognizing that 2D materials present a key opportunity for polaritonics, demonstrating in 2015 the first strong light–matter coupling in 2D materials (Liu et al., 2015). The published work on photonic properties of 2D materials opened a new field as evidenced by full sessions at major conferences such as the Conference on Lasers and Electro-Optics (CLEO) and smaller workshops dedicated to the topic of strong light–matter coupling in 2D materials. In 2015, Dr. Gerhold took two additional actions to pursue polaritonics. First, he organized a 2015 IEEE Photonics Society Summer Topical plenary presentation on breakthrough work from room temperature gallium nitride (GaN) polariton lasers. Second, he joined Dr. Marc Ulrich, the Solid State Physics Program Manager, to fund a low-temperature GaAs effort to assess “polaritonics”—polaritonic circuit concepts—with state-of-the-art epitaxial microcavities. These combined efforts revealed to Drs. Gerhold and Ulrich the opportunity to move the field forward through a large multidisciplinary effort. The two issued a Multidisciplinary University Research Initiative (MURI) topic to pursue polaritonics in 2D materials and competitively selected the University of Michigan to lead the effort. Encouraged by Dr. Gerhold to pursue additional collaborations, the University of
One of Professor Menon’s most recent advances enabled by ARO’s investments is his group’s demonstration of Rydberg states of excitons in 2D semiconductors to realize highly nonlinear polaritons. Rydberg excitonic states, like in atoms, are highly excited electronic states with relatively large size (Bohr radius). The larger size allows stronger interparticle interactions, thereby increasing their nonlinear response. Indeed, this approach of using Rydberg states has been used with much success in cold atomic gases to realize single photon switches and for exploring many-body phenomena. The work by Professor Menon’s group was the first time that Rydberg states were used to enhance nonlinear optical interactions to unprecedented levels in solid-state systems. They took advantage of the presence of highly stable excitons in semiconducting 2D transition metal dichalcogenides (TMDs), a recently discovered class of materials in the semiconductor arena. Owing to their high binding energy (strength with which the excitons are held together), the Rydberg states of these excitons are spectroscopically accessible even as high as liquid nitrogen temperature (77 K). This allowed the Menon group to realize Rydberg exciton-polaritons, a first by itself using monolayer tungsten diselenide, an archetypal TMD embedded in a microcavity, as shown schematically in Figure 5. In the work, published in Nature Communications (Gu et al., 2021), they showed that the state of the microcavity device can be switched with just ~100 photons. While this is still classical optics, it is an important step toward quantum nonlinearity as well as for realizing highly efficient attosecond switches. Indeed, an immediate application of these highly nonlinear polaritons is in implementing optical reservoir computing architectures.

Another recent result from the Menon group in the context of engineering nonlinearity under the MURI effort was the realization of a large second-order nonlinear response from self-hybridized polaritons that form in bulk 2D materials (several layers) without the need for external mirrors (Figure 6). This is one of the first demonstrations of a strong second-order nonlinear response from a bulk centrosymmetric crystal. This goes against the conventional textbook picture; symmetry precludes second-order nonlinear response in bulk centrosymmetric crystals. However, in this case, strong coupling occurs without the need for a cavity due to the Fabry–Perot resonances that arise from the large refractive index contrast close to the excitonic resonance. Intriguingly, the strongly coupled bulk TMD system demonstrates higher second-harmonic generation efficiency than its monolayer counterpart. This occurs because the asymmetric electric field decouples the layers (i.e., the bulk crystal acts as a collection of individual layers with a non-vanishing second-order response). This work, which is currently under review, has implications not just for second-order effects, but also for higher harmonic generation and all-optical signal processing. High harmonic generation enables much higher-energy light for unique sensing modalities. All-optical signal processing promises extraordinary efficient and fast information processing.

**WAY AHEAD**

A natural extension of this work is to consider functional exciton-polaritons in other 2D materials. Likewise, the stage is set to study new device concepts employing these nonlinear phenomena. It will be particularly important to have access to large-area 2D materials, determine ways to integrate them with suitable optical cavities, and devise novel concept device structures suitable for taking advantage of the nonlinear optical structures for emitters, detectors, and photonic computing concepts.
SOLID-STATE ELECTRONICS AND ELECTROMAGNETICS PROGRAM

Program Manager
Dr. Joe Qiu

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 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 DEVCOM ARL in 2008 as an Electronics Engineer and then to ARO in 2013 as the Program Manager for Solid-State Electronics and Electromagnetics.

Current Scientific Objectives

1. Discover and create unique electromagnetic phenomena in solid-state materials and structures that require theoretical formulations beyond well-established Maxwell's equations that, if successful, will create new types of electrically tunable microwave/millimeter-wave/terahertz devices.

2. Create novel device concepts based on emerging phenomena in heterostructures and interfaces of engineered quantum materials that, if successful, will enable future electronic systems with significantly lower size, weight, and power and higher information processing capacity.

3. 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 that, if successful, will potentially enable beyond-5G wireless communications in this part of the electromagnetic spectrum.

SUCCESS STORY

Laughing Gas Laser: Widely Tunable Compact Terahertz Gas Lasers with Nitrous Oxide

Army-funded researchers from the Harvard University John A. Paulson School of Engineering and Applied Sciences (SEAS), in collaboration with the Massachusetts Institute of Technology (MIT) and the U.S. Army, have developed a compact, room-temperature, widely tunable terahertz laser using nitrous oxide (commonly known as laughing gas) as the gain medium. This laser will open a large, underused region of the electromagnetic spectrum and pave the way for better sensing, imaging, and communications.

CHALLENGE

The terahertz part of the electromagnetic spectrum has remained out of reach for most applications. That is because current sources of terahertz frequencies are bulky, inefficient, have limited tuning, or must operate at low temperature. For example, one of the earliest sources of terahertz radiation is optically pumped far-IR (OPFIR) lasers. However, OPFIR lasers are inefficient and large (~1 m), and require an equally large carbon dioxide (CO$_2$) laser and high-voltage power supply. Moreover, they are poorly tunable, requiring the lasing gas and CO$_2$ laser line to be changed each time a different frequency is needed.

ACTION

Dr. Henry Everitt, a senior scientist at DEVCOM AvMC at the time, had studied molecular spectroscopy throughout his career and realized that broad terahertz tunability could be made possible by using a continuously tunable mid-IR pump source such as a quantum cascade laser (QCL) in place of a CO$_2$ laser. A tunable QCL can optically pump almost any roto-vibrational transition of almost any molecule, thereby promoting population from lower level into a virtually empty excited vibrational level to facilitate lasing at a broad range of frequencies. Furthermore, comprehensive physics-based multilevel models of the dominant collisional processes in gas molecules with a permanent dipole moment show that OPFIR lasers can operate efficiently in compact cavities with volumes more than 10$^3$-fold smaller than conventional cavities.
Professor Federico Capasso of Harvard, who co-invented QCL at Bell Laboratories in the 1990s, had a serendipitous encounter with Dr. Everitt at a conference where they realized they could use a widely tunable pump like the QCL to make a broadband terahertz laser. Professor Capasso was excited by the new idea and the possibility of a powerful and broadly tunable terahertz source. He and Dr. Everitt explained the idea to Dr. Qiu, Program Manager of ARO’s Solid-State Electronics and Electromagnetic Program. Because of the program’s objective to develop new capabilities at the terahertz frequencies for future Army broadband communications and radar applications, the proposal was compelling. This unique proposal combined Dr. Everitt’s deep knowledge in molecular spectroscopy and Professor Capasso’s expertise in novel, compact laser sources. Dr. Qiu subsequently decided to fund the proposed work as a cooperative agreement to facilitate the collaboration.

**RESULT**

Their breakthrough, called the QCL-pumped molecular laser (QPML), is characterized by frequency tunability over the entire range of rotational transitions from the molecular gas gain medium. Broad terahertz tunability is made possible by using a continuously tunable mid-IR QCL as the pump source. Powerful, portable QCLs are capable of efficiently producing widely tunable light. The theory to optimize the operation of the new laser was developed by Professor Steven Johnson, MIT; his graduate student Fan Wang; and Dr. Everitt.

The researchers combined the QCL pump with a nitrous oxide (aka laughing gas) laser (Figure 1). By optimizing the laser cavity and lenses, they were able to produce frequencies spanning nearly 1 THz. Nitrous oxide offers broad tunability over 37 lines spanning 0.251 to 0.955 THz, each with kilohertz line widths. Analysis shows that laser lines spanning more than 1 THz with powers greater than 1 mW are possible from many molecular gases pumped by QCLs. Thus, Professor Capasso and Dr. Everitt exceeded the expectations of their original idea of a QCL-pumped broadband terahertz laser.

Heterodyne receivers were used to measure the spectrum of these laser transitions. The instantaneous line widths were <1 kHz, but because of frequency jitter, the effective line widths were typically 3 to 6 kHz. The researchers were able to demonstrate frequency tuning of the laser across its full Doppler-broadened gain bandwidth by precisely adjusting the cavity length with a motorized micrometer (Figure 2). Importantly, the QPML frequency was quite stable (routinely <10 kHz) while freely running and could be made even more stable through active frequency stabilization of the QCL and the laser cavity.

A comprehensive theoretical model was able to estimate the collisional cross sections and predict the optimal performance of the laser. For a given QCL pump power, the terahertz power achievable by this room-temperature laser depends on several factors. A three-level model, which takes into account the very low-pressure regime in which molecular collisions with the chamber walls occur more frequently than any intermolecular collisions, captures the salient behavior.

The research was published in the journal Science (Chevalier et al., 2019).

**WAY AHEAD**

The concept of QPML is universal for all polar gas molecules. Lasing can be induced on any dipole-allowed rotational transition by sufficient pumping of a related roto-vibrational transition using a continuously tunable QCL. The Harvard team and their Army collaborators will continue to explore other gases as gain mediums to achieve even broader tunability and higher output power. As reported in the Science paper (Chevalier et al., 2020):

*Results*

- Published in the prestigious journal Science.
- Realized a new QPML concept for a compact, broadly tunable terahertz laser.
- Demonstrated a tuning range of nearly 1 THz with laughing gas.

*Anticipated Impact*

This research is expected to open a large, underused region of the electromagnetic spectrum for high-bandwidth communications, ultra-high-resolution imaging, precise long-range sensing for radio astronomy, and much more.
"Molecular THz lasers pumped by a quantum cascade laser offer high power and wide tuning range in a surprisingly compact and robust design," said Nobel laureate Theodor Hänsch of the Max Planck Institute for Quantum Optics in Munich, who was not involved in this research. "Such sources will unlock new applications from sensing to fundamental spectroscopy."

“What’s exciting is that concept is universal,” said Paul Chevalier, a postdoctoral fellow at SEAS and first author of the paper. “Using this framework, you could make a terahertz source with a gas laser of almost any molecule and the applications are huge.”

This laser could be used in everything from improved skin and breast cancer imaging to drug detection, airport security, and ultrahigh-capacity optical wireless links.

SUCCESS STORY

Giant Topological Longitudinal Circular Photogalvanic Effect

Army-funded researchers at the University of Pennsylvania have demonstrated that there is a topological origin of the ability of cobalt monosilicide (CoSi) to convert light into electrical current. This could provide a new approach for developing devices such as photodetectors, solar cells, and efficient terahertz sources.

CHALLENGE

The dependence of photocurrent in a material on the light’s polarization is known as the circular photogalvanic effect (CPGE). Transverse CPGE, where the current flows perpendicular to the light propagation direction, is by far the most commonly observed. It has been measured in transition metal dichalcogenides, topological insulators, and Weyl semimetals.

In contrast, the longitudinal CPGE, where current flows parallel to the light propagation direction, could be quantized because it arises from nontrivial topology and could reveal unique insight of crystal geometry. Since its initial discovery in tellurium in 1979, longitudinal CPGE remains elusive and has not been demonstrated in other materials. Chiral topological semimetals feature protected nodal crossings near the Fermi level, and because all mirror symmetries are broken, nodes with opposite chirality generically appear at different energies, in contrast to mirror-symmetric Weyl metals, like tantalum arsenide (TaAs), with nodes at the same energy. The existence of these nodes is protected by an integer topological charge C, which could lead to quantized longitudinal CPGE.

Chiral Weyl metals, where C = ±1, have not been found. However, separated topological nodes with degeneracies larger than 2, known as multifold fermions, have been demonstrated to exist in chiral crystals such as CoSi, rhodium silicide (RhSi), and aluminum-platinum (AlP) (with C = ±4). Moreover, the presence of cubic symmetry in these materials makes transverse CPGE vanishing and longitudinal CPGE isotropic.

ACTION

Relatively recent theoretical developments in topological materials revealed that under certain conditions, Maxwell’s equations, which govern electromagnetic radiation, should be modified. These advances suggested that when electromagnetic radiation passes between a topological material and a non-topological material (such as air or a vacuum), the effect—referred to as axion electrodynamics—would be observable. Dr. Qiu invested in research by Professor Peter Armitage at Johns Hopkins University to observe this effect using terahertz spectroscopy. As a result, Professor Armitage and his then student, Liang Wu, established the first direct experimental evidence for axion electrodynamics and the associated topological magneto-electric effect. Because of this, Professor Wu received the 2017 Richard Greene Dissertation Award in Experimental Condensed Matter Physics by the American Physical Society, the 2019 William McMillan Award for outstanding contributions in condensed matter physics, and the 2020 Macronix Prize. Due to his excellent track record, Dr. Qiu selected Professor Wu for an ARO Young Investigator award to further pursue terahertz and nonlinear terahertz effects in related materials with the objective of determining their suitability as a new platform for faster memory devices and energy-efficient optoelectronic applications.

RESULT

Professor Wu and his students used terahertz emission spectroscopy to investigate longitudinal CPGE in CoSi (Figure 3). The CPGE was measured by detecting radiated terahertz pulses emitted from regions illuminated by the short laser pulses, a method with several advantages compared to DC current measurements. First, detecting CPGE in a contactless way avoided contact misalignment as
CHAPTER 3  
SUCCESS STORIES

Results

- Published in the prestigious journal Nature Communications.
- Realized the longitudinal photogalvanic effect in CoSi was purely topological in origin.
- Discovered the photocurrent of CoSi in the mid-IR regime was higher than what had previously been observed in other types of materials with chiral structures.

Anticipated Impact

This discovery could provide a new approach for developing devices such as photodetectors, solar cells, and efficient terahertz sources using topological materials.

Professor Wu developed the capability to measure terahertz emission in the low-energy mid-IR regime (0.20–0.48 eV) for the first time. This enabled him to measure CPGE in CoSi across a broad range of 0.2–1.1 eV. He identified a large longitudinal photocurrent peaked at 0.4 eV reaching ~550 µA/V², which was much larger than the photocurrent in any chiral crystal reported in the literature. Comparing the measurements to first-principles calculations, the peak was identified to originate from topological band crossings, reaching 3.3 ± 0.3 in units of the quantization constant under the assumption of a constant hot-carrier lifetime. A theoretical model that took into account quadratic corrections to the dispersion of the nodal bands was developed and showed that the location of the chemical potential could lead to a more complex frequency profile than it had been anticipated even in the spinless model. These calculations also laid out the conditions to observe the quantized CPGE in CoSi in future experiments.

The research was published in the journal Nature Communications (Ni et al., 2021).

WAY AHEAD

Through their latest findings, Professor Wu and his team now have the experimental procedures and analytical methods in place to study other types of materials and phenomena that could be relevant for materials science and engineering applications. By using a combination of both experiment and theory, these results also have further implications for improving topological materials for more widespread use in the future. As reported in Ni et al. (2021):

“This is an experimental demonstration people are trying to associate with a topological character that may well be in the observed properties if we can make the materials a little better, and I think that’s really being done here for the first time,” said Professor Eugene Mele, University of Pennsylvania.

“Right now, the materials aren’t quite there, but it looks like they could be. And that is a pretty amazing idea.”

In addition to understanding its topological origin, the very large photocurrent of CoSi in the mid-IR regime could pave the way for using topological materials to create high-sensitivity photodetectors and high-efficiency terahertz sources.
Dr. Evan Runnerstrom completed his undergraduate studies at Stanford University, receiving his B.S. in 2009 and M.S. in 2010 in Materials Science and Engineering. 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 Materials Design.

SUCCESS STORY

ARO Investments in Self-Assembly Lead to New 3D-Printed, Multifunctional Metamaterials

An ARO-sponsored researcher is creating new, multifunctional materials through the design and self-assembly of molecular crystals. These molecular crystals combine multiple functionalities—ferroelectricity, magnetism, and/or energetic decomposition—in one tunable system, opening the door for future Army technologies based on soft, conformable, and dynamic functional materials.

CHALLENGE

A longstanding challenge in the materials science community is to impart designed functional properties, such as magnetism, conductivity, and ferroelectricity, into molecular materials such as polymers or crystals of small molecules. While these functional properties are abundant in solid-state materials like perovskite oxide ceramics, the rigidity and processing requirements for solid-state materials limit their utility toward Warfighter-relevant applications like conformal coatings, flexible materials, or 3D printing. Moreover, the broad design space offered by molecular materials would enable the design of multifunctional materials with multiple active constituents. If these constituents are periodically arranged in a crystal, their electronic properties can combine to enable multiple functions within the material, such as multiferroic behavior that combines ferromagnetism, ferroelectricity, and/or ferroelasticity. Materials with simultaneously tunable magnetic, dielectric, elastic, and electronic properties are key to the Army’s efforts in creating dynamic materials for future technologies like extreme low-power computers, extreme-density memory and logic circuits, and highly precise electronic and magnetic sensors.
However, achieving such behavior in solution-processed, self-assembled molecular crystals is no easy feat—the available design space can be overwhelmingly large, it can be difficult to achieve crystallization of multiple constituents, and precise self-assembly and materials design strategies are needed to achieve the proper coexistence and coupling of electronic and magnetic order to achieve multiferroic behavior.

**ACTION**

ARO Materials Design Program Manager Dr. John Prater (now retired) recognized the challenges and opportunities for soft, self-assembled materials like molecular ferroelectrics. In an effort to reconnoiter a potential pivot from the Materials Design Program’s then-emphasis on conventional or “hard” materials like perovskite oxides toward soft materials, Dr. Prater organized a 2011 workshop titled “Directed Self-Assembly of Materials Workshop.” Present at that workshop was Shenqiang Ren, now a Professor of Mechanical Engineering at the University of Buffalo. Dr. Prater and Ren were already familiar thanks to an ARO-managed Multidisciplinary University Research Initiative (MURI) project that supported Ren’s graduate work at the University of Maryland. Like Dr. Prater, Ren’s interests were shifting from conventional ferroelectrics to molecular, self-assembled soft materials systems. After extended discussions during and following the workshop, Dr. Prater invited a proposal based on organic photovoltaic materials for the Young Investigator Program (YIP), which was awarded to Professor Ren in 2015.

Following the conclusion of that award, Dr. Runnerstrom worked to continue ARO’s support of Professor Ren’s research under a Single Investigator (SI) grant titled “Molecular Design and Assembly Towards Conducting Ferroic Crystals.” This proposal was notable for its aims to create new smart materials that combine multiple ferroic functionalities using a 3D crystalline charge transfer concept—rational combination of electron donor and electron acceptor groups in molecular crystals. This proposal idea circumvented the aforementioned challenges by creating molecular crystals that self-assemble through long-range noncovalent attractions. Professor Ren also proposed to leverage advances in machine learning and molecular informatics to shrink the “search space” of donor and acceptor molecules capable of crystallization. Throughout the YIP and SI grant, Drs. Prater and Runnerstrom have facilitated Professor Ren’s collaboration with a number of researchers in DEVCOM ARL WMRD.

**RESULT**

Under the current ARO grant, Professor Ren has achieved multifunctional behavior in a number of molecular systems and form factors, and is making steady progress toward achieving full multiferroic behavior in self-assembled molecular systems. Along the way, Professor Ren has published a number of notable papers in high-impact journals detailing his materials design approach to imbue molecular crystals with multiple functionalities:

- “Strongly Correlated Molecular Magnet with Curie Temperature above 60 K,” published in Matter. In this work, Professor Ren demonstrated the growth of iron–tetracyanoquinodimethane (FeTCNQ), a layered compound with strong electronic coupling among the charge, electron spin, and crystal lattice. This material realizes a number of useful properties, such as magnetism and light-induced conductivity.

- “Emerging Magnetic Interactions in van der Waals Heterostructures,” published in Nano Letters. Similar to the previous report, here Professor Ren showed how (Li,Fe)OHFeSe, another layered molecular compound, displays a superconducting ground state thanks to hydroxide intercalation. Intercalating additional electron donating molecules within the layered structure induced strong, tunable magnetic behaviors, as well as the ability to generate conductivity via laser illumination. Both this and the work with FeTCNQ demonstrate that properly designed layered compounds offer excellent potential as hosts for coupled electronic and magnetic properties, a crucial stepping stone toward molecular multiferroics.

- “A 3D-Printed Molecular Ferroelectric Material,” published in the Proceedings of the National Academy of Sciences (PNAS). This landmark result builds on previous work, done in part by Professor Ren, to show that imidazolium perchlorate (ImClO₄) is a robust molecular ferroelectric material. Molecular ferroelectrics are particularly useful for responsive 3D metamaterials because their reversible electric polarization enables tunable dielectric and elastic properties. The key advance was to develop a 3D-printing process that enabled the creation of the first 3D molecular metamaterials to simultaneously display ferroelectricity, transparency, and self-healing ability. This work paves the way for new classes of tunable vibration damping and tunable electronic materials that can be easily and scalably integrated with existing systems via 3D printing.

**Citations (con’t):**


**Results**

- Led to an ARO workshop, YIP award, and SI grant in a new area of research combining self-assembly and multifunctional, multiferroic materials design.

- Demonstrated initial success in a molecular crystal design that enabled combined electronic, magnetic, and optical functionalities in self-assembled, layered molecular crystals.

- Discovered a new molecular ferroelectric material, ImClO₄, along with a route to creating 3D metamaterials of crystalline ImClO₄ using additive manufacturing approaches. These metamaterials have tunable electronic, dielectric, and mechanical properties, and have promise as scalable and tunable vibration damping materials for the Army.

- Discovered that ImClO₄ combines ferroelectricity and energetic properties in a single material, with detonation velocities comparable to TNT, and showed that the energetic decomposition of ImClO₄ simultaneously generates a burst of electricity.
This success was made possible by:
Dr. Evan Runnerstrom,
Materials Science Branch

Citations:

WAY AHEAD
Professor Ren and DEVCOM ARL collaborators will next apply machine learning and related design tools to identify other promising molecular candidates that combine multiple functionalities. This will not only lead the way to new energetic ferroelectrics with improved performance, but also to true molecular multiferroic materials, the ultimate goal of this project. To make these materials attractive for future energetic, ferroelectric, and multiferroic applications in the Army, the team will also work to scale candidate materials to large areas at low cost by further exploring 3D printing and other additive manufacturing approaches.

SUCCESS STORY
New Data-Driven Approaches for Computer-Aided Design of Soft Matter
A new ARO-sponsored researcher is exploring machine-learning-empowered simulation techniques for faster, predictive modeling of soft matter and self-assembling materials. Generalized models for soft matter systems, like polymers and colloids, will likely be useful for designing and building multifunctional and reconfigurable systems for the modern Army.

CHALLENGE
Two grand challenges of soft matter research are to link functional properties and behavior with the underlying multiscale structure, and discover generalized forward and inverse design rules to create soft matter systems with desired emergent and/or dynamic functionality. Tackling these challenges requires the ability to understand and control mesoscale structures, processes, and dynamics over length scales ranging from atoms to bulk materials and over timescales ranging from nanoseconds to minutes. This profound requirement is notoriously difficult to achieve with existing computational strategies for modeling soft matter—methods that capture atom-level accuracy are too computationally expensive, while mesoscale methods like coarse graining do not accurately address the true complexity, breadth, and emergent properties of soft matter, which are, of course, what make soft materials special.

ACTION
While on a site visit to the University of Wisconsin in 2019, Dr. Runnerstrom took the opportunity to meet with Wenxiao Pan, an Assistant Professor of Mechanical Engineering with ongoing research interests at the intersection of soft matter, computer simulation, and machine learning. Professor Pan explained her ideas to create a new, data-driven, coarse-graining method that circumvents the existing shortcomings.
of coarse graining and machine learning (e.g., ad hoc approaches that are different for each system and non-transferable). Success would result in a new paradigm for soft matter modeling, where predictive dynamic simulations would be both computationally viable and highly accurate. After discussing these ideas at length, both in person and on the telephone, Dr. Runnerstrom encouraged Professor Pan to develop a full proposal on the topic. Upon further realizing that Professor Pan would be a first-time DoD grantee, Dr. Runnerstrom informed Professor Pan of her eligibility for a Defense Established Program to Stimulate Competitive Research (DEPSCoR) grant and encouraged her to apply.

RESULT

Per the DEPSCoR application requirements, Professor Pan applied with a collaborator previously funded by the DoD (Professor Kaibo Liu, a machine-learning expert at Wisconsin). Their grant application, titled “Mesoscale Modeling of Soft Matter: A Bottom-up Approach,” received excellent reviews and was one of three DEPSCoR proposals chosen by the DoD Basic Research Office for a three-year, $600,000 grant. Professor Pan’s strategy is to use select all-atom molecular dynamics simulations as a training ground to build up mesoscale coarse-grained models that combine atomic fidelity with the ability to simulate soft matter over multiple time and length scales, starting with true atomistic descriptions of diverse soft matter systems like polymers and colloids with no ad hoc approximations. Using strict mathematical and statistical mechanics theory, Professor Pan is establishing the nonstationary Langevin equation (nsGLE) as a dynamic equation of motion that fully describes the static/equilibrium and dynamic/nonequilibrium properties of a soft matter system over any time and length scale and without approximation. The nsGLE is an important construct, because it incorporates dynamic macroscopic and microscopic variables, and is used to describe Brownian motion—a critical aspect of self-assembly and molecular simulations.

In the first year of their DEPSCoR project, Professors Pan and Liu have made significant progress executing this strategy, with two publications in Soft Matter. One of these publications, “Transfer Learning of Memory Kernels for Transferable Coarse-Graining of Polymer Dynamics,” was highlighted as the journal’s cover article for the June 2021 issue. The “memory kernel” is a component of the nsGLE that influences the dynamics of a system over all timescales and preserves fidelity under coarse graining. If one knows the memory kernel at a time $t$, then the state of the system can be accurately predicted at any preceding or subsequent time $t'$. The memory kernel is difficult to determine explicitly—the key advance by Professors Pan and Liu was to show that the memory kernel can be inferred using training data and contemporary machine-learning techniques like Gaussian process regression. Through careful application of statistical mechanics and active learning theory, this result also showed that the memory kernel can be transferred to other systems to enable predictions outside of the training dataset, which is normally a major weakness of machine-learning methods. The potential impact of this approach for computer-aided materials design is significant when one considers that it enables one to predict the time-dependent dynamic properties of soft materials under different thermodynamic (e.g., temperature) and geometric (e.g., polymer chain length) conditions, even if those parameters are not within the initial training dataset.

WAY AHEAD

Professor Pan is working to further develop her data-driven, coarse-graining strategy in order to apply the technique to a broader swathe of soft matter systems. A prime example is in active soft matter systems, sometimes called active matter or dissipative systems, which consume energy to dynamically self-assemble or reconfigure to achieve desired functional properties. To properly model these active systems, additional effort will be needed to properly choose the coarse-graining variable to represent nonequilibrium processes like externally applied forces or fluid flows. Dr. Runnerstrom is working to involve interested Army scientists as potential transition partners for this work. Advanced soft matter modeling techniques like coarse graining could dramatically enhance the design of protection materials or dynamic color-changing materials based on soft matter systems like polymers and colloids.

Figure 2: (left) Soft Matter journal cover image highlighting the transferable coarse-graining process. (right) Atom-level representation of a peptoid polymer to be simulated, along with a plot comparing the diffusion dynamics of the polymer as simulated by the coarse-graining technique and all-atom molecular dynamics.

ARL Competencies:

- Sciences of Extreme Materials
- Photonics, Electronics, and Quantum Sciences
- Mechanical Sciences

Results

- Secured one of three available ARO DEPSCoR grants to bring in an assistant professor new to the DoD research ecosystem.
- Established a new, collaborative soft matter research project that combines mathematically rigorous statistical mechanics with machine learning to create new coarse-graining techniques that maintain accuracy and provide for transferability across multiple soft materials systems.
- Led to two publications, including a cover article, demonstrating that so far this approach is feasible and can enable accurate predictions of polymer behavior, even under conditions that are outside of the training data.

Anticipated Impact

New generalized, accurate, and transferable coarse-graining and machine-learning techniques have the potential to revolutionize the ability to design and predictively model dynamic soft materials. This new simulation paradigm will contribute to the Army’s modernization efforts by dramatically reducing the time needed to develop new soft materials and integrate them into systems for adaptive protection, dynamic color- and shape-changing coatings, and soft robotics.
MECHANICAL BEHAVIOR OF MATERIALS PROGRAM

Program Manager
Dr. Daniel Cole

Dr. Cole completed his undergraduate studies at the State University of New York College at Geneseo, receiving his B.S. in Physics in 2004. He received his Ph.D. in Mechanical Engineering from the University of Maryland in 2009.

He came to ARO in 2019 as the Program Manager for Mechanical Behavior of Materials.

Current Scientific Objectives

1. Discover material phenomena that enable extreme mechanical behaviors through dramatic improvements in energy dissipation, toughness, stiffness, hardness, and resiliency (to include new understanding, control, or confinement of deformation mechanisms; exploitation of heterogeneous material systems and interface/interphase interactions to enable unprecedented properties while avoiding inherent subsystem weaknesses; and novel approaches for materials to perform in extreme thermomechanical environments) that, if successful, would enable new technologies for Soldier and vehicle protection, advanced propulsion systems, and hypersonic applications.

2. Investigate structural materials that actively respond to dynamic loading environments and other external stimuli through rapid adaptation of shape, topology, or mechanical properties (to include mitigation or manipulation of stress wave propagation, novel actuation schemes that generate extraordinary forces or require minimal input energies, and novel material responses initiated through multiaxial loading) that, if successful, would enable unprecedented capabilities for protection, maneuver, and reconfigurable systems.

SUCCESS STORY

Exploiting Ripplocations to Enable Layered Materials with Tunable Strength and Toughness

This effort has given the Army understanding of how competition between deformation mechanisms in layered structures may enable materials with extraordinary combinations of mechanical properties. This work is expected to enable impact- and wear-resistant materials, as well as coating technologies for extreme operating environments.

CHALLENGE

A challenge often encountered in the materials design community is being able to improve a specific property without compromising another important property. For example, in many composite systems, strength may be increased with respect to the neat matrix (e.g., pure epoxy) by introducing stiff fillers (e.g., carbon fibers), but this often comes at the expense of toughness (e.g., introducing aligned carbon fibers in an epoxy matrix will greatly increase the load capacity in particular directions, but often this causes the material to be relatively brittle). Heterogeneous material systems are attractive because properties may be tuned and multifunctionality may be introduced; yet, engineers traditionally have to consider tradeoffs that may be unacceptable for implementing in real design scenarios. Thus, many materials scientists seek novel routes to avoid these tradeoffs and realize desirable mechanical properties without the non-desirable material behaviors.

ACTION

Given the importance to numerous Army technologies, materials with unusual combinations of mechanical properties have long been of interest to the Mechanical Behavior of Materials (MBM) Program. Starting in 2011, an ARO-funded Single Investigator (SI) effort at Drexel University was investigating strength and toughness associated with nanoscale materials. In 2016, the group reported on a previously unknown deformation mechanism that was seen in a layered structure. The group had performed indentation...
In 2018, ARO invited a white paper from Professor Tucker, now at the Colorado School of Mines, to study how rippllocations in nanoscale laminates with varying layer thicknesses could be exploited to enable unprecedented combinations of strength and toughness. The principal investigator teamed with an experimentalist, Professor Sid Pathak at Iowa State University, to investigate how rippllocations in certain layers and other types of deformations in neighboring layers could instigate a “competition” between mechanisms that could enable new tools for tuning mechanical performance and, crucially, realize desirable behaviors without compromising other important properties.

Given the potentially foundational discoveries made during the first two years of the grant, the MBM Program recommended an instrumentation award to the team in 2020. The equipment consisted of a micromechanical testing system capable of performing compression, bending, tension, and indentation on micrometer-scaled specimens. In addition, the system has the capability for testing over a range of temperatures (150 to 1000 °C) and strain rates (10^-4 to 10^4 s^-1), which is allowing the team to explore the performance of these composite laminates in the extreme operating environments of interest to the Army.

**RESULT**

The team proposed investigating a metal/MAX phase nanolaminate (here, M is an early transition metal, A is typically a group 13-16 element, and X is carbon and/or nitrogen, which results in a stable metallically bonded laminate). The team initially focused on understanding this complicated mechanical behavior in titanium aluminum carbide (Ti1.3AlC.) and titanium silicocarbide (Ti2.5SiC.) MAX phases through atomistic simulations, which were previously impossible given the lack of bonding information for these materials. The group developed interatomic potentials for the materials and constructed model systems that could then be subjected to simulated mechanical loading to observe the resulting deformations. The models showed how initial buckling behaviors self-align into rippllocation boundaries (RBs). The RBs were shown to be reversible up until the point at which the ripples become pinned, delaminate from neighboring layers, and, in areas of maximum strain, form permanent buckles known as “kink-bands” (KBs) (Figure 1).

Here, the A-layers (black in the figure) act as ball bearings, as the MX-layers elastically deform over the A-layers. The kinked structures allow for additional energy absorption, which the team hypothesized could increase the toughness of the composite without sacrificing other important mechanical behaviors (e.g., strength).

To validate the simulations, the team experimentally tested a single grain of a zirconium aluminum carbide (Zr1.3AlC) nanolaminate through an indentation experiment. An electron-transparent foil was extracted from the indented sample and imaged using scanning tunneling electron microscopy (STEM). The STEM image revealed a main delamination area in the material; atomic resolution imaging revealed a KB with distinct delamination cracks on either side (Figure 2). These results indicated that the atomistic simulations were capturing the correct strain accommodation processes in the metal/MAX phase composites.

The team has explored several metal/MAX compositions to further test the range of mechanical behaviors that may be achieved through this approach. The group fabricated micropillars of the nanolaminates and has performed indentation studies to assess the improvement in mechanical behaviors with respect to the individual metal or MAX phases. Initial experimental studies on niobium (Nb)-Ti1.3AlC and Ti-Ti1.3AlC systems have indicated large increases in strength (i.e., 200-400%) with respect to the MAX phase, while also

**Results**

- Used atomic-scale simulations to uncover a nanoscale buckling behavior in layered materials, which provides a new mechanism to dissipate energy.

- Showed, via experiments on metal/MAX layered nanocomposites, large increases in strength (e.g., 200-400%) with respect to individual layers without sacrificing toughness.

**Anticipated Impact**

Understanding the ways in which deformation mechanisms “compete” within layered materials is expected to enable future leap-ahead technologies for Soldier and vehicle operation in extreme environments.
This success was made possible by:

Dr. Dan Cole,
Materials Science Branch

Dr. David Stepp, ARO Chief Scientist

Citations:


... retaining much of the ductile behavior of the metal phase and avoiding the typical tradeoff of strength versus toughness. The relative thickness of the metal/MAX layers has been shown to activate certain deformation modes, while suppressing other mechanisms, which may yield new tools for designing materials with a desired response. Future experiments will further investigate the layer thickness question, as well as the properties of the materials at various strain rates and temperatures.

This effort may give Army engineers new tools for designing materials with extraordinary combinations of mechanical properties. Armor, aerospace structures, and propulsion system coatings all require combinations of properties to perform in extreme environments, but are difficult to achieve within a single material. More broadly, the kinking behavior mechanisms that are being investigated in this study are thought to occur in a variety of natural (e.g., mica, ice, wood, geological formations) and engineered (e.g., laminated composites) materials, which indicates that these results may have scale independence and therefore be applicable to a variety of layered systems.

WAY AHEAD

In the last year of this effort, the team will characterize various metal/MAX nanocomposites using a micromechanical test platform with in situ heating and cooling and variable strain rate capabilities, which was part of an ARO Defense University Research Instrumentation Program (DURIP) award in 2020. These tests will help establish the suitability for these materials to perform in extreme thermomechanical operating environments.

SUCCESS STORY

Extreme Energy Dissipation Behaviors in Liquid-Crystal Elastomers

This research has provided a new understanding of how molecular alignment may be programmed into liquid-crystal elastomers (LCEs) to enable extraordinary mechanical energy dissipation. The effort is expected to provide new ballistic protection technologies, vibration damping strategies, as well as novel actuators for soft robotics applications.

CHALLENGE

Extreme mechanical energy is found all over the battlefield and thus the Soldier requires materials that can effectively absorb and safely dissipate this energy.

For example, intense vibrations from rotorcraft systems, vehicle collisions, and impacts from ballistic events pose significant challenges for Soldier safety and vehicle sustainability. Current technologies often add parasitic mass (e.g., vehicle dampers, bulky body armor, etc.), which will hinder the future expeditionary Soldier. The goal for this project was to develop a fundamental understanding of the relaxation mechanisms of LCEs to enable tunable, mechanical, energy-dissipative behaviors.

ACTION

A major thrust for the MBM Program in 2016 was on force-activated materials. This included novel materials design strategies to tailor failure mechanisms to mitigate the propagation of intense stress waves and control energy dissipation. Discussions with a team led by Professor Vicky Nguyen at Johns Hopkins University (JHU), who was collaborating with a group at the University Colorado Denver (CU Denver), explored the possibility of using stimuli-responsive materials known as LCEs for extreme energy dissipation.

The team proposed to investigate programmed molecular alignment in LCEs and the resulting effects on mechanical energy dissipation over multiple length scales; this project was funded starting in 2017.

In 2018, a site visit and project review was organized at JHU. A DEVCOM ARL staff researcher working with the MBM Program as a tech advisor was invited to attend, which led to discussions of synergistic activities at DEVCOM ARL focused on the multiaxial vibrational response of aero-structures. The MBM Program coordinated a DEVCOM ARL-Aberdeen Proving Ground visit for the JHU/UC Denver team to tour the laboratories and discuss potential experiments on LCEs to assess energy-dissipative behaviors in response to multiaxial vibrations. This led to the JHU/UC Denver team sending samples to DEVCOM ARL for evaluation. The DEVCOM ARL group had a test fixture instrumented in-house for imposing the...
vibrations and used a digital image correlation setup to evaluate the mechanical response. DEVCOM ARL then hired a graduate student in the co-principal investigators’ group at CU Denver for a summer 2020 internship to further investigate the suitability of these materials for damping in rotorcraft structures.

RESULT

LCEs are composed of stiff molecular components known as mesogens, which are bound in a flexible network. The mesogens may rotate relative to the network chains, which may give rise to a variety of interesting thermomechanical behaviors, such as actuation, as well as temperature-, frequency-, and loading rate-dependent energy dissipation. These effects can be even more dramatic if the mesogens are incorporated into the backbone of the polymer chain (i.e., “main-chain” LCEs), as opposed to configurations on the branches of the polymer chain (i.e., “side-chain” LCEs). The main-chain configuration offers a high degree of chain anisotropy (i.e., direction-dependent material properties that could be exploited for tuning the mechanical response in particular orientations and vastly different responsiveness in other orientations). The given study sought to exploit the microscopic and macroscopic mesogen ordering in the main-chain configuration to enable extreme mechanical energy-dissipative behaviors.

The team used a recently developed method for processing main-chain LCEs through a “click reaction” that featured a UV light crosslink step that allowed the mesogen alignment to be “locked-in.” This step also allowed the group to explore short- and long-range mesogen ordering: (1) “polydomains” consisting of local mesogen order on the size of micrometers but globally in a disordered state and (2) “monodomains” consisting of mesogens entirely aligned over the bulk material. The main-chain LCEs were stretched to various degrees and then exposed to the photopolymerization process. The team specifically looked at 0% strain that explored the mesogens in the polydomain state, medium strains that corresponded to partial monodomain states, and large strains that resulted in the monodomain state, and then used wide-angle X-ray scattering to quantify the various degrees of mesogen ordering. The LCE samples were then subject to a variety of mechanical tests to better understand the mesogen relaxation mechanisms at various lengths scales. The team found this stretching-induced “locked-in” structure could be used to control the strain rate dependency of these materials; for example, the LCEs pre-stretched to 90% of the full monodomain state displayed a much weaker strain rate dependency with respect to the polydomain LCEs. The monodomain samples displayed much higher degrees of anisotropy given the global mesogen ordering. These results were important because they may provide tools for materials engineers to design the optimal damping response of a structure for applications at various strain rates.

In addition to extreme energy dissipation, the group also discovered new ways to control the mechanics of the deformation process. For example, the team demonstrated that the polydomain samples deform through nonuniform strain behaviors that could be exploited to design specific local and global responsiveness.

Figure 3 shows the strain heterogeneities that develop in polydomain LCEs. Using digital image correlation, the group characterized the full-field strain behaviors at various rates. The inset in top left shows a representative stress–strain curve highlighting four key areas in the mechanical response: (1) starting point for softening, (2) strain softening region, (3) strain hardening region, and (4) maximum stretch. For lower strain rates (Figures 3c and 3d), the samples displayed horizontal bands of relatively high strains during the initial softening, and a pattern of alternating bands of high/low strain was observed during the strain stiffening. At faster rates (Figures 3a and 3b), this effect was not as pronounced in the strain softening region, but was eventually observed near the maximum stretch. These results were attributed to strain bands forming from polydomain relaxation, which were more pronounced at lower strain rates.

There are a number of Army applications being considered for this work. The team has worked with DEVCOM ARL in-house scientists to study the highly anisotropic damping behaviors at various frequencies in order to assess the capability for LCEs to serve as multifunctional vibration damping structures for air and ground vehicles. The team has incorporated the LCE resins into an additive manufacturing process known as digital light processing (DLP), and has demonstrated processing of complex geometries, including lattice structures, and even lotus flowers. The LCE lattice structures were shown to have 12 times greater rate-dependence and up to 27 times greater strain-energy dissipation compared to those printed from a commercial photocurable elastomer. The group has also 3D printed an LCE-based spinal cage using the porous lattice architecture, which demonstrates the potential for fabricating mechanical energy-dissipating medical devices. In addition, the DEVCOM Soldier Center has issued an award to the co-principal investigators’ startup company, Impressio Inc., to 3D print the LCEs for combat helmet liners.

WAY AHEAD

DEVCOM ARL has run preliminary studies on the multiaxial vibration response of the LCE materials to investigate multifunctional structures with inherent damping behaviors. In addition, DEVCOM Soldier Center has recently awarded a contract to a company started by the co-principal investigators to develop combat helmet liners using 3D-printed LCEs.

ARL Competencies:

- Sciences of Extreme Materials
- Terminal Effects
- Mechanical Sciences

Results

- Demonstrated LCEs with high energy dissipation controlled over various length scales and directionality and 3D-printed LCE lattices with 27 times strain energy dissipation with respect to commercial elastomers.
- Led to a graduate student funded under this effort being hired by DEVCOM ARL for a 2020 summer internship.
- Performed dynamic mechanical tests on LCE membranes at DEVCOM ARL to assess damping behaviors in response to vibrations for potential rotorcraft sustainability applications.
- Led to the co-principal investigators being awarded a contract with DEVCOM Soldier Center to 3D print LCE energy absorbers for combat helmet liners.

Anticipated Impact

Hierarchical control of molecular units can be used for extreme mechanical energy dissipation applications, and may enable new technologies for lightweight Soldier protection and damage adaptive vehicles.
**SUCCESS STORY**

**Two-Dimensional Covalent Organic Frameworks with Extraordinary Thermal Properties**

Two-dimensional organic polymers (covalent organic frameworks [COFs]) were discovered, for the first time, to have extraordinary thermal properties. These results were made possible due to collaborations between a Multidisciplinary University Research Initiative (MURI) team and Single Investigator (SI) awardees established by proactive action taken by ARO Program Manager Dr. Varanasi.

**CHALLENGE**

With the recent advances made in electronic device designs and electronic materials, miniaturization of energy-efficient devices continues to improve. However, there is an increasing need for materials with extraordinary thermal properties, such as low-dielectric constant but high thermal conductivity, for thermal management of novel devices to function properly and increase reliability. Novel thermal management materials are expected to limit the electronic crosstalk, signal propagation delay, and charge buildup that often reduce the functionality of devices. Novel COFs belong to such a class of novel thermal management materials that have a low dielectric constant and layered periodic structures that could offer extraordinary thermal properties. However, challenges associated with characterizing conventionally isolated polycrystalline COF powders have restricted the exploration of many 2D COF thermal properties.

**ACTION**

In 2015, Dr. Varanasi initiated a MURI program in collaboration with Dr. Dawanne Poree, Polymer Chemistry Program Manager, to discover and synthesize 2D organic polymers, commonly known as COFs. The principal investigator of this project is Professor Will Dichtel from Cornell University/ Northwestern University. The team consisted of researchers from chemistry and physics disciplines from the Georgia Institute of Technology, University of California, Berkley, Cornell, and Northwestern.
This team mainly worked toward developing novel chemistries and 2D COF film synthesis routes and discovering their electronic properties. The MURI team also collaborated with Dr. Eric Wetzel’s group at DEVCOM ARL WMRD to explore the mechanical properties of these novel materials films as additional add-on efforts of the MURI. Significant advances were made in the synthesis and mechanical and electronic property characterization of these materials by this MURI team. However, the thermal properties of these materials were not investigated due to a lack of expertise available in the MURI group.

Dr. Varanasi’s Physical Properties of Materials Program also covers the thermal properties of materials as one of its focus areas. He has been funding SI and MURI programs to discover novel materials with extraordinary thermal properties and novel phenomena, as well as develop novel characterization techniques to determine thermal properties. Some of the notable programs initiated include near-field thermal radiation, spin caloritronics, thermal conductivity of novel materials such as chalcogenides, super-atomic crystals, and thermal transport across interfaces between different materials. Because of these interactions with the thermal community, he introduced the COF MURI team to the SI awardees of the Physical Properties of Materials Program: Professor Patrick Hopkins (University of Virginia), who is an expert in thermal property characterization, and Professor Alan McGaughey (Carnegie Mellon University), who is an expert in thermal modeling. Due to the proactive action taken by Dr. Varanasi to establish collaborations between the MURI team, who are experts in the chemical synthesis of novel materials, and the SI grantees of thermal community, a new discovery was made possible, as explained in this Success Story.

RESULT

The researchers from the MURI team and SI grants have collaborated and reported fabrication of high-quality COF films, which enabled thermoreflectance and impedance spectroscopy measurements (Figure 1). They found that 2D COFs exhibit unusually high thermal conductivities (1 W m\(^{-1}\) K\(^{-1}\)) for low-density, low-k dielectrics, achieving a dielectric permittivity of 1.6 (Figure 2). This is a combination of properties that is a prerequisite for next-generation integrated circuits. These results show that oriented, layered 2D polymers are promising next-generation dielectric layers and that these molecularly precise materials offer tunable combinations of useful thermal, electronic, and mechanical properties. These results were published in Nature Materials.

WAY AHEAD

These results have been shared with DEVCOM ARL scientists. Drs. Poree and Varanasi are collaborating to initiate new programs (SI, MURI, or Small Business Technology Transfers) to further develop these novel COFs for active thermal management. These programs will explore the material parameters that influence the thermal conductivity and dielectric permittivity of COFs and various mechanisms for active thermal management. If successful, these COFs would be well suited for thermal management of future electronics or heat signature reduction devices. Future plans will explore opportunities to collaborate with the Energy Sciences Competency as well as Sciences of Extreme Materials Competency at DEVCOM ARL to enable tech transition.
SUCCESS STORY

Novel Method to Reduce Losses in Thermophotovoltaics and Other Advances in Near-Field Thermophotovoltaics

A novel method to reduce losses in far-field thermophotovoltaics (TPVs) using an air bridge behind a photovoltaic (PV) cell was developed. Also high-efficiency thermal-to-electrical energy conversion using a near-field TPV configuration and novel materials was demonstrated for the first time.

CHALLENGE

TPVs convert thermal energy into electrical energy using an emitter and a PV cell. Far-field TPVs have been investigated for many years, and recently, significant advances are being made using high-temperature photonic crystals. However, novel approaches such as near-field TPVs, which take advantage of near-field evanescent modes, are relatively unexplored. In the near field, the emitter and PV cells are separated by a very small gap distance that is less than the wavelength of the emitted radiation, allowing higher rates of heat transfer. Near-field TPVs are being actively explored now due to their potential for high-power-density and high-efficiency energy conversion. However, progress toward functional near-field TPV devices has been limited by challenges in creating thermally robust planar emitters and PV cells designed for near-field thermal radiation.

In addition, to reach high efficiencies, TPV cells must utilize the broad spectrum of a radiative thermal source. However, most thermal radiation is in a low-energy wavelength range that cannot be used to excite electronic transitions and generate electricity. One promising way to overcome this challenge is to have low-energy photons reflected and reabsorbed by the thermal emitter, where their energy can have another chance at contributing toward photogeneration in the cell. However, current methods for photon recuperation are limited by insufficient bandwidth or parasitic absorption, resulting in large efficiency losses relative to theoretical limits.

ACTION

In 2012, Dr. Varanasi identified a new scientific opportunity to explore materials that enable radiative heat transfer in nanoscale dimensions. At that time, most of the research was conducted in nanoscale conductive heat transfer, but little attention was paid to radiative heat transfer in the nanoscale. He started a SI grant with Professors Pramod Reddy and Edgar Meyhofer of the University of Michigan to explore near-field radiative heat transport (NFRHT) between parallel surfaces of different materials. In this project, experimental verification of near-field radiation theories that are more than 70 years old was obtained. Seeing the success of this result, a multi-principal investigator (Professors Reddy, Meyhofer, and Steve Forrest) project was started in 2017 to unravel underpinning mechanisms in near-field-based radiative heat transfer and energy conversion processes utilizing novel thin films and heterostructures. Such basic research efforts are initiated to operationalize the fundamental scientific results. For example, a fundamental understanding is necessary to realize high-efficiency TPV cells for converting thermal energy into electrical energy. In 2019, Dr. Varanasi also initiated a MURI project in collaboration with Dr. Marc Ulrich, currently of the Electronics Branch, to further explore near-field phenomena in even narrower gaps, where theories are yet to be developed. The MURI team (principal investigator Professor Reddy) started exploring the fundamental principles of NFRHT phenomena such as NFRHT in ångström-sized gaps (i.e., sub-nanometer extreme NFRHT [eNFRHT]), and NFRHT between non-reciprocal, nanostructured 2D and phase-change materials, as well as novel near-field energy conversion phenomena. DEVCOM ARL’s continued support for more than a decade has helped to shape and advance the field of near-field radiation and associated phenomena.

RESULT

Professor Forrest’s team at University of Michigan, part of the MURI effort, demonstrated near-perfect reflection of low-energy photons by embedding a layer of air (an air bridge) within a thin-film indium gallium arsenide (In$_{0.53}$Ga$_{0.47}$As) cell (Figure 3). This result represents a fourfold reduction in parasitic absorption relative to existing TPV cells. The resulting gain in absolute efficiency exceeds 6%, leading to a very high power conversion efficiency of more than 30%, as measured with an approximately 1,455-K silicon carbide emitter. These results were published in Nature.

The MURI team led by Professor Reddy also demonstrated a record power density of ~5 kW/m² at an efficiency of 6.8% in a near-field TPV system, where the efficiency of the system is defined as the ratio of the electrical power output of the PV cell to the radiative heat transfer from the emitter to the PV cell (Figure 4). This was made possible by this multidisciplinary team of experts aimed at developing novel emitter devices that can sustain temperatures as high as 1,270 K and positioning them into the near field (~100 nm) of custom-fabricated InGaAs-based, thin-film PV cells. In addition to demonstrating efficient heat-to-electricity conversion at a high power density, this team also reported the performance of TPV...
Results

• Demonstrated record-breaking energy conversion performance for a near-field TPV device.
• Published in Nature and Nature Communications.
• Led to research collaborations with DEVCOM ARL SEDD.

Anticipated Impact

High-efficiency energy conversion devices may enable expeditionary power sources for Soldiers in the future that operate at low temperatures and are capable of utilizing various heat sources including waste heat.
Dr. Bakas obtained his Ph.D. in 2006 in Materials Science Engineering from Rutgers University, and did research on armor materials and their processing at the Idaho National Laboratory for eight years. He has been the Program Manager for Synthesis and Processing of Materials for five years.

SUCCESS STORY

Integrated Computational and Experimental Approaches for the Discovery of Advanced Materials Launched in Support of Science of Extreme Materials Competency Goals

Dr. Bakas coordinated discussions between extramural researchers and DEVCOM ARL scientists and engineers by conducting workshops under the auspices of the Science of Extreme Materials (SEM) Competency to identify basic research thrusts that could support Competency goals to operationalize science for transformational overmatch. From these discussions, a need for basic research into computational approaches for discovering novel new materials was identified. Dr. Bakas invited competitive proposals and made a case for two new extramural grants that propose innovative research in this area.

CHALLENGE

Most computational methods base their predictions on the relatively well-understood criteria of thermodynamic equilibrium, but cannot predict the numerous metastable phases that can occur on the path to equilibrium. In addition, the nearly unlimited potential compositions available make it nearly impossible to use trial-and-error experimental methods to identify metastable materials, as the time and expense required are prohibitive. Thus, to start being able to predict metastable materials, it is necessary to develop an experimental/computational strategy with clearly defined criteria that can enable strong synergy between the computational and experimental aspects.

ACTION

The role of the Synthesis and Processing of Materials Program, in the framework of the DEVCOM ARL SEM Competency, is to identify and support extramural basic research that will make possible the long-term goals of the Competency. Based on discussions initiated by SEM Competency leads Dr. Ernest Chin (intramural) and Dr. Chakrapani Varanasi (extramural), Dr. Bakas identified a need to develop an increased capability to identify new material options via computational means. Most computational methods are based on thermodynamic equilibrium, which is mathematically defined and supported by a vast library of data. However, many useful metastable materials exist in nonequilibrium states but can be retained due to kinetic forces. Tools for predicting the existence of these materials are much more limited, and additional basic research is needed to advance them.

To determine the best investments to make, Dr. Bakas arranged a workshop between extramural principal investigators and DEVCOM ARL researchers to discuss the fundamental challenges in this
area. The attendees realized that extramural efforts on this topic should focus on discovering materials with beneficial phase mechanisms, as these are most likely to lead to a disruptive new material. The principal investigators also suggested that more investments in the understanding of kinematics might improve the ability to predict metastable materials. Kinematics governs what atomic pathways are available to reach equilibrium, and understanding these pathways enables potential identification of transitory or metastable phases (Levitas et al., 1998). Finally, a need to create Bayesian priors based on established physics might enable more rapid materials discovery. These Bayesian priors would eliminate potential outcomes that violate known physics, reducing computational costs.

In addition, it was recognized that more active collaboration among ARO, DEVCOM ARL, and the extramural principal investigators was needed to enable transition of code from computationally based extramural efforts to DEVCOM ARL. Coordination with DEVCOM ARL researchers needs to be established to ensure data and code can be readily transferred and applied to internal research. There are solutions already in place that could be employed to enable such transfer, such as GitHub, which could enable this type of code sharing.

**RESULT**

Having identified specific technical directions to address the challenge of computational prediction, Dr. Bakas was able to solicit two new proposals focused on these challenges. One of these was a joint effort by Professor Christopher Schuh of the Massachusetts Institute of Technology (MIT) and Professor Srikanth Patala of North Carolina State University. This proposal was focused on discovering ceramic materials that exhibit the shape memory effect. Shape memory is when a material reverses any deformation once a certain temperature is reached. This reversal is caused by a specific type of phase transformation that occurs, called a martensitic transformation (Otsuka et al., 1999). In a martensitic transformation, atoms move via shear from one position in a crystal structure to another. This shear transformation (as opposed to the more common diffusional transformation) causes the material to physically change shape. In the case of shape memory materials, this causes it to revert to its previous shape, undoing any deformation.

While shape memory has been demonstrated in metal alloys, all attempts to induce shape memory effects in ceramics have caused cracking. Professors Schuh and Patala believe that it might be possible to create a viable shape memory zirconia-based ceramic material. The zirconia composition would need to be altered to satisfy the established criteria laid out by previous researchers for a viable shape memory material (Chen et al., 2013) and also minimize the volume mismatch between the two phases of the transformation. This second criterion is not needed for ductile metals, but is necessary for brittle ceramics to avoid cracking. Professors Schuh and Patala proposed an integrated experimental and computational effort to design the shape memory ceramic. Past experimental data and data in the literature were used to perform the initial computational predictions of the ideal composition. These identified titanium (Ti) and aluminum (Al) as possible dopants to use to achieve the desired volume mismatch. Experiments were then conducted on the identified range of compositions, and the cracking in the zirconia ceramic was greatly reduced (Figure 1). The data obtained from the experiments will be used to adjust the next simulations. These adjusted simulations will then be used to guide the next experimental efforts, until the exact composition where all criteria are met is found. Not only will this research potentially identify a material with a beneficial phase transformation mechanism, the understanding of kinematics will be advanced as well. Shape memory ceramics would be excellent materials for high-stress and high-temperature applications such as hypersonic munitions.

![Figure 1: Zirconium dioxide (ZrO2)-titanium dioxide (TiO2)-aluminum oxide (Al2O3) ceramic composition that demonstrates reduced cracking with compositional adjustment.](image)

The second project was put forth by Professor Axel van de Walle of Brown University. Professor van de Walle was hoping to expand on the ability to predict metastable phases computationally by identifying the range of potential energy states that could exist for specific conditions. For calibration, Professor van de Walle will be using a collection of experimental data of unusual “mazed microstructures” created at the Lawrence Berkeley National Laboratory (Radetic et al., 2012). These microstructures cannot be predicted computationally with current methods, and a simulation that can predict their formation will enable prediction of other nonequilibrium grain boundaries and microstructures. Professor

**Discussed potential new materials with a unique mechanical response (shape memory ceramics) for future use in hypersonics and other applications.

• Added a future capability to more accurately and quickly predict the existence of metastable materials, enabling more rapid discovery of new material options.

**Anticipated Impact**

The shape memory effect could provide a potential means of mitigating damage in future ceramic materials, which are often used in aerospace and protective applications. An enhanced ability to predict metastable phases could enable discovery of new material options with better performance for meeting modernization needs.
van de Walle will also be developing Bayesian priors for the thermodynamic parameters governing the phase transformations involved. Figure 2 shows an example, where the crystal structure is used to make predictions of the viable surface energy configurations, enabling more rapid prediction of the surface morphology that will occur upon crystallization.

As these efforts provided key contributions for the long-term goals of the SEM Competency, Dr. Bakas put them forth as candidates for potential Congressional funding. This request was supported by Drs. Varanasi and Chin of the SEM Competency, who recognized how the projects would advance SEM goals. The projects were initiated as Cooperative Agreements to enable future sharing of the code and data generated with DEVCOM ARL researchers.

WAY AHEAD

With the Cooperative Agreements established, DEVCOM ARL researchers will interface with the new efforts. These interactions will be necessary to facilitate the future sharing of the code and data that results. Drs. Bakas, Varanasi, and Chin will visit MIT and Brown to understand the progress and explore tech-transfer opportunities coming out from these efforts.

SUCCESS STORY

Improved Methods for High-Temperature Material Fabrication through International Collaboration

The Synthesis and Processing of Materials Program Manager, Dr. Bakas, has successfully initiated collaborations with the International Division Program Managers, and identified two research efforts for the creation of high-temperature alloys and composites that are resistant to creep. The first project, a joint effort between Northwestern University (NU) and EMPA in Switzerland, explored fabrication of high-temperature oxide dispersion strengthened alloys via additive manufacturing, and a second effort at the Institute of Science and Technology for Ceramics in Italy (ISTEC) will explore the more flexible processing of high-temperature ceramic composites in support of the Army Modernization Priorities of Soldier Lethality, Next Generation Combat Vehicle, and Future Vertical Lift.

CHALLENGE

Creep, the deformation of material under high temperatures and constant stress, is one of, if not, the limiting factor for materials used in aerospace applications. However, many of the materials capable of resisting creep can only be fabricated by methods with inherent drawbacks or costs that create limitations on the use of these materials. New fabrication strategies that are more flexible and amenable to production are needed to enable more widespread adoption of these materials, but the focus of ARO Program Managers on domestic research institutions means capabilities developed internationally might be overlooked.

ACTION

One option for high-temperature, creep-resistant materials is oxide dispersion strengthened (ODS) nickel (Ni)-based superalloys, metal alloys that use refractory oxide particles to strengthen performance at high temperatures. Past ODS alloys had to be fabricated via powder metallurgy, as other methods would cause the loss of many of the particle strengthening mechanisms that make ODS alloys effective. Dr. Bakas became aware of research that might enable more flexible fabrication of high-temperature materials through the then Materials International Program Manager Dr. Julie Fife. At the EMPA (Swiss Federal Laboratories for Materials Science and Technology), Dr. Christian Leinenbach had created a new Ti-based ODS alloy that could be rapidly melted and solidified while still retaining an effective oxide dispersion (Kenel et al, 2017). This made it potentially suitable for more advanced fabrication methods such as additive manufacturing (AM). In addition, EMPA had a first-rate AM lab, capable of not only producing samples, but also studying the building process and microstructures via an in situ synchrotron micro-focused X-ray analysis system capable of capturing high-resolution data regarding the thermal cycles and phase transformations occurring during the AM process. This instrument gave EMPA an ability to characterize the AM process in a manner that not many other institutions could match.
Dr. Bakas thought it would be a good practice to pair the international researcher with a domestic research institution with more experience working with the DoD. Working with the new International Division Program Manager Jim Harvey, Dr. Bakas encouraged a proposal in which EMPA partnered with Professor David Dunand of NU. NU has unique atom probe and modeling capabilities that would help design the alloys. The Synthesis and Processing of Materials Program supported a grant to design and test additively manufactured ODS superalloys.

Another opportunity to develop a different type of high-temperature materials was made available when Dr. Amanda Napier, Technical Director of International Technology Center (ITC)-South Europe, called Dr. Bakas’ attention to work being done in Italy. ISTEC participated in a large European Union project called C3HARME, in which they developed a number of high-temperature ceramic-matrix composites (Zoli et al, 2017a, 2017b). Work on the C3HARME project gave the ISTEC researchers an in-depth expertise in the fabrication of ceramic composites that could not easily be replicated. An example of these composites, a high-temperature carbon fiber–zirconium diboride composite, is shown in Figure 3. The researchers proposed to develop a more flexible fabrication approach for these materials, employing classic liquid phase sintering methods. Liquid phase sintering involves introducing additional materials that melt and form a liquid that enables the composite to fully consolidate. Dr. Bakas encouraged an emphasis on studying the behavior and design of the liquid phase, as while this method is effective in densifying a material, the remnants of the liquid phase could degrade high-temperature performance.

RESULTS

The NU/EMPA project utilized unique X-ray imaging characterization tools developed at EMPA to capture critical data about the builds. A Ni-chromium (Cr)-Al-Ti superalloy was developed and printed, using both hafnium and yttrium oxides for the particles (Kenel et al, 2021). In addition, ODS Al-zirconium (Zr) superalloys were developed that were printed and tested for creep performance. These alloys showed high creep resistance, demonstrating an ability to additively manufacture an ODS alloy without losing the particle strengthening mechanisms, an important milestone for establishing the viability of these materials. This creep resistance is demonstrated by Figure 4, where the ODS alloys deform 8 to 10 times slower at 800 °C. The grant has produced three publications with four more pending.

Dr. Luca Zoli of ISTEC submitted a proposal addressing the liquid phase sintering of ceramic composites and found a partner in Professor William Fahrenholtz of the Missouri School of Science and Technology (MS&T), who has great experience in ceramic processing and is willing to help evaluate the new potential materials. In addition, Dr. Napier was able to convince the Office of Naval Research (ONR) to invest some support for the project, and active collaboration with ONR researchers is expected as the program gets underway. This is another example of how international engagement can enable the DoD to leverage results generated from international efforts like the C3HARM effort to research that will support its own goals.

WAY AHEAD

As the NU/EMPA effort reaches a conclusion, a potential new program will be explored of developing new refractory AM alloys for potential use in hypersonic and other aerospace applications. In addition, an attempt to tie the effort more directly to DEVCOM ARL internal research in this area will be pursued. The ISTEC-MS&T project is being launched soon as a Cooperative Agreement is in place and should begin shortly into FY22. Further fruitful international collaborations will be pursued in coordination with ITC and ARO’s International Programs.

Figure 3: Hot-pressed carbon fiber-reinforced zirconium diboride high-temperature ceramic composites.

Figure 4: Creep testing at 800 °C with (a) vertical stress and (b) horizontal stress. The ODS alloys have a significantly reduced strain rate (creep) over time compared to the base alloy. The slope changes in the rate correspond to different creep mechanisms, from grain boundary sliding $n = 1.2$ to dislocation glide $n = 5$.

ARL Competencies:

• Demonstrated the ability to 3D print creep-resistant ODS alloys.

• Led to a new Cooperative Agreement to develop ceramic processing for high-temperature ceramic composites.

Anticipated Impact

The development of processing methods for the creation of creep-resistant materials that could be employed in aerospace and hypersonic applications.
COMPLEX DYNAMICS AND SYSTEMS PROGRAM

Program Manager
Dr. Dean Culver

Dr. Culver began his academic career at Duke University studying high-dimensional dynamical systems and applied nonlinear dynamics with Professor Earl Dowell supported by a grant from ARO. He also worked with the Office of Naval Research on metamaterial design as well as passive and active wave manipulation during his graduate career. Since then, Dr. Culver has made contributions in nonlinear structures, biomechanics, and molecular biophysics.

After completing a postdoctoral fellowship with VTD at DEVCOM ARL, he accepted a civilian research position with ARL WMRD before ultimately moving into the Program Manager for Complex Dynamics and Systems at ARO.

Current Scientific Objectives

1. Expand the 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 that, if successful, will lead to a broad range of future capabilities (e.g., novel energetic and entropic transduction, agile motion, and force generation).

2. Understand how information, momentum, energy, and entropy are directed, flow, and transform in nonlinear systems due to interactions with the system’s surroundings or within the system itself that, if successful, will enable advances in robotics, vehicle design, munitions, energy storage, and power sources.

3. Push beyond a 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 that, if successful, will promise disruptive innovations in robotics, vehicle design, munitions, energy storage, and power sources.

SUCCESS STORY
Emergent Matter from Assembly of Micron-Scale Atomic Origami Robots

Professor Itai Cohen and his team at Cornell University have changed the answer to the question, “What is the smallest possible robot we can control while empowering it to locomote and manipulate its environment?”

Using novel fabrication techniques and recent advancements in our understanding of electroactive nanomaterials, this effort has produced the first sub-100-μm robot featuring onboard processing.

CHALLENGE

This effort had a number of obstacles to overcome to realize these novel devices. One of them was fast, repeatable, and controllable actuation at the nanoscale—a problem that required exploration of the electrochemistry of shape-memory structures. A streamlined series of capabilities to support this exploration into micron-scale robotic devices did not exist before this effort either, as there was no need to test and examine a system that was just theoretical. The final major hurdle the team overcame involved a fabrication procedure for onboard computing. The team developed a clever light-driven system that could be integrated onto incredibly small surfaces while providing the memory necessary for individual robots to carry out a wide array of functions.

ACTION

These new devices and the fundamental scientific advances necessary to enable them are the consequence of collaborative efforts from a team of different ARO Program Managers and their foresight over a number of years. In addition to accurately forecasting and precisely identifying when an area of
science is “ripe” for advancement based on the collision of clever theories circulating through the literature in disconnected arenas and novel experimental techniques to validate them, the previous Complex Dynamics and Systems Program Manager, Dr. Sam Stanton, and colleagues within ARO invited and encouraged proposals in active matter, emergent behavior from micron systems, and more. Almost equally as importantly, efforts have ramped up to transition results from this effort into DEVCOM ARL’s intramural portfolio, including higher technical readiness level (TRL) efforts, as it is clear that the scientific advancements fueled by ARO’s work have established new engineering capabilities. This includes connecting Professor Cohen with Drs. Todd Henry and Asha Hall of DEVCOM ARL to brainstorm Army applications for collaborative micron-scale devices in both the deep and even near future.

RESULT

One of the most impactful results of these efforts is the characterization and engineering of graphene glass bimorphs. By patterning extremely thin (2 μm) rigid panels on top of these bimorphs, the team was able to localize bending to unpatterned regions to produce bidirectional folds for origami structures. This means that reliable micron-scale actuators with incredible geometric versatility are a reality. To drive home how incredibly small these folds can be and how much authority engineers could have over the design of sub-micron actuation, the team set a world record for the smallest origami crane ever folded (Figure 1). The team has also integrated nanoscale origami actuators with simple electronics, namely, photovoltaics. These results showed the micron robots can be powered and controlled using standard complementary metal–oxide–superconductor (CMOS) electronic components like photovoltaics and transistors. Using this technology, first sub-100-μm robot that integrates onboard electronics was created (Figure 2).

Since then, the project investigated many nuances of the material involved in the bimorphs. Results showed that platinum-based actuators could be operated at high enough voltages that oxygen undergoes place exchange reactions with the platinum that are not thermodynamically irreversible. This means that the actuators can retain shape memory, making them “programmable” for specialized functions. Additional ongoing efforts include integrating a CMOS-based timing circuit with a cilial array to demonstrate a viable platform for artificial cilia, which allows the same engineering principles that enabled microscale robots to develop disruptive microfluidic device capabilities. The team is prepared to publish a comprehensive report on a CMOS-integrated robot that is capable of locomotion, phototaxis, and receiving commands. Finally, Professor Cohen and his colleagues are fabricating even stronger actuators made either of nickel or palladium, offering more applications of the new microbots.

These results were published in manuscripts in high-impact journals such as Proceedings of the National Academy of Sciences, Advanced Materials, Science Robotics, and Nature.

WAY AHEAD

This is an excellent example of a crossroads where a fundamental scientific effort spun off a new technological capability. The fundamental scientific investigation (understanding of and authority over surface electrochemistry) led to the realization that incredibly strong and even more incredibly tiny sheets of material could be quickly and repeatably deformed on command. This realization collided with state-of-the-art, optically controlled processors on a similar scale to create a robot capable of sensing, exploring, and manipulating environments in ways the scientific and technological communities have never been able to. What’s more, these robots can communicate with each other and other devices. While the original intent of this effort was to explore emergent phenomena associated with hosts of these robots, their current capabilities suggest Army applications beyond the deep-future notion of devices-made-of-devices. And this deep-future potential cannot be overstated. Camelia Bacchus of SmallCapNews summarizes this very effectively.

Results

- Led to actuators that let us explore and manipulate microscale environments, the world’s smallest programmable robot, and advancements in surface electrochemistry (paving the way for novel material and active matter design).

Anticipated Impact

This effort may lead to a potential near-future reconnaissance tool, which is a big step forward on the road to programmable systems of systems. Broadly impactful advancements in surface electrochemistry offer progress in the field of active matter.
In her March 18, 2021, report on Professor Cohen’s work, she writes, “Imagine a million microscopic robots free from a chip that bends, breaks free, and performs its tasks, even as it assembles more complex structures. This is the vision.” But in the near term, exploring and expanding the capabilities of this generation of robots could result in an extremely cost-effective reconnaissance tool. Next steps include connecting Professor Cohen and his team to intramural investigators to brainstorm additional applications and determine what resources could be directed to developing near- and deep-future Army capabilities. It is important to acknowledge that this new tool is the consequence of sustained support for fundamental scientific efforts in surface electrochemistry, materials science, and especially complexity.

### SUCCESS STORY

#### From Information Theoretic Control and Learning to Nonequilibrium Stochastic Thermodynamics

This Success Story demonstrates imparting creative decision-making into control systems and robots, and correctly identifying when the seeds of such a capability (in terms of personnel and the scientific tools to validate correct theories) were ready to take root. Solicitations in this area, fostering talented individuals with great ideas, and relationships between intramural researchers and extramural partners came together to build a framework for adaptability in vehicles and robots. The largest success here is a direct collaboration between Dr. Brett Piekarski in DEVCOM ARL’s intramural research and Professor Evangelos Theodorou of the Georgia Institute of Technology on adaptability and creative decision-making for one or more vehicles, and a substantial contribution to Dr. Piekarski’s Scalable Adaptive and Resilient Autonomy (SARA) and Distributed and Collaborative Intelligent Systems and Technology (DCIST) Cooperative Research Agreements (CRAs).

#### CHALLENGE

Before these efforts, a framework for approaching the daunting task of improving the efficiency of learning and controllers in autonomous systems was largely piecemeal. It was becoming increasingly clear that conventional deep learning techniques were insufficient for guiding the behavior of autonomous systems reacting to short-timescale anomalies. In these instances, the uncertainty associated with measurements of the environment is quite high. Thus, reactive or model predictive control are necessary (Figure 3). But these control schemes are not mature, and what’s more, the underlying science of information flows in uncertain systems is incomplete.

Certainly, advances in deep learning and reinforcement learning have led to impressive gains in the control of real-world systems with complex nonlinear dynamics and in the ability to analyze video and other noisy high-dimensional data to extract actionable information about the world. These successes have led to renewed optimism about the ability to tackle the fundamental problem in artificial intelligence (AI): the ability to learn causal models that connect perception to action and support real-time autonomous decision-making in complex problem domains such as robotics, social media, and cybersecurity. The success of current deep architectures comes from their ability to extract highly specialized feature representations from large amounts of data. While they have demonstrated substantial performance gains, they have a number of limitations that must be addressed: (1) inability to efficiently incorporate prior knowledge, (2) inability to represent uncertainty, (3) lack of modular and reusable components, and (4) difficulty in capturing causal dependencies.

There’s another approach that can be taken to ask the question, How do we create efficient learning and control systems for autonomous systems reacting to sudden stimuli? Like many other fields of engineering, dynamicists and control engineers are turning toward highly effective examples of adaptation and versatile capability in nature. Many biological systems we see feature distributed controllers, morphology fairly specific to the tasks of a given component, and adaptation/learning. In this behavior–morphology–computation triumvirate (shown and expressed with a little more detail in Figure 4), how can computational thermodynamics be characterized, and what is the role of uncertainty and nonlinearity in these systems?
ACTION

The story begins with a 10-year-old ARO Multidisciplinary University Research Initiative (MURI): “Neuro-Inspired Adaptive Perception and Control for Agile Mobility of Autonomous Vehicles in Uncertain and Hostile Environments.” Although the primary monitor for the MURI was former ARO Program Manager Dr. Alfredo Garcia, Dr. Sam Stanton (the then Complex Dynamics and Systems Program Manager) supported the work as well. Among the many fantastic outcomes of the MURI was a notion that characterization of uncertainty and bounding the high-dimensional space of machine-learning algorithms for adaptation using predictive models could improve the algorithms’ effectiveness. Dr. Stanton worked with Professor Theodorou (one of the performers in the MURI) to organize a conference on this subject that included many expert academics from universities across the country. The results of this conference and the engagement from the community fueled by successful, ARO-managed research through the MURI program included a draft framework that had eluded the controls community up to that time. The Complex Dynamics and Systems Broad Area Announcement (BAA) entry was updated to include language to solicit proposals and efforts within this framework in order to enable the adaptive and versatile robots necessary for future Army application.

RESULT

The primary result of these efforts is the alignment of extramural research in the roadmap to real-time adaptive autonomy to the goals of DCIST and SARA. This is formalized in the direct collaboration between Dr. Piekarski in DEVCOM ARL and Professor Theodorou in the effort entitled “Perceptual Decision Making Architectures for Single- and Multi-Vehicle Coordination,” but that does not fully capture the consequences of networking Professor Theodorou and his colleagues with DEVCOM ARL researchers. The workshop entitled “The Statistical Physics of Stochastic Optimal Control and Learning” spawned new efforts from investigators across the country, many of which now fall under the DCIST or SARA CRAs. The scientific merit of these projects cannot be overstated. Collecting these notions of the thermodynamics of computation and quantifying their relationship to a device’s (or an organism’s) morphology as well as the environment under the heading of “information-theoretic control” is a crucial step in exploring and characterizing future control paradigms in extremely high-dimensional and uncertain spaces.

WAY AHEAD

By continuing to champion basic scientific topics to support the SARA and DCIST CRAs and the roadmap to efficient control for autonomous robots in uncertain environments established by the ARO-supported conference mentioned previously, the Complex Dynamics and Systems Program is streamlining progress toward autonomous Army robots in the battlefields of tomorrow. In the more immediate term, ongoing extramural research in this space includes advancements in several subareas, including (but not limited to) the following:

- The development of stochastic control algorithms for large-scale systems as well as systems with spatiotemporal dynamics. These classes of systems include processes that can be represented by infinite-dimensional diffusions and stochastic partial differential equations or systems that can be represented by a large set of stochastic differential equations (SDEs). Such systems can be found in fluid mechanics, soft robotics, and large-scale multi-agent systems.

- The development of information-theoretic stochastic control algorithms using generalized entropies. In addition, generalization of these algorithms for systems with stochasticities. Application of these algorithms include systems in autonomy, robotics, and applied physics.

- Generalization of information-theoretic stochastic control and path integral control algorithms to open quantum systems under different observation protocols. Open quantum systems are represented by SDEs, making this subject a perfect candidate for applied information-theoretic control. The ultimate goal is generalization of the entire stochastic optimal control theory and its connections to statistical physics for the cases of open quantum systems.

- Using ideas from stochastic control and nonequilibrium statistical mechanics to develop new algorithms for learning representations. These representations may include either physics-based models of dynamical systems in autonomy, robotics, and applied physics or general machine-learning representations.

ARL Competencies:

- Mechanical Sciences

Results

- Developed a roadmap to adaptive and versatile Army robots of the deep future.
- Led to soaring engagement with the DCIST and SARA CRAs.
- Led to direct collaboration between the Georgia Institute of Technology and intramural DEVCOM ARL researchers.
- Developed clear guidelines for future work in adaptive and learning robotics within the ARO portfolio.

Anticipated Impact

Autonomous robotic design capable of learning and adaptation could arise from advancements in fast and efficient stochastic control.
Dr. Julia 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 Earth Materials and Processes.

SUCCESS STORY
Unearthing Real-Time 3D Ant Tunneling Mechanics

Motivated by the desire to improve our own ability to dig underground—be it for mining, tunnels, or waste disposal—a team of researchers from the California Institute of Technology (Caltech) has unraveled one of the secrets behind how ants build their amazingly complex and stable structures. Led by the laboratory of Professor José Andrade (Caltech), the team studied the digging habits of ants and uncovered the mechanisms guiding them. The research is described in a paper published in the journal Proceedings of the National Academy of Sciences.

CHALLENGE
Professor Andrade, an expert in granular materials, was intrigued by the complex structure ants form as they create their underground cities. Although beneath the surface, castings of ant nests have shown that the structures are large and impressive.

Desire to understand load bearing in tunnels and the ability to identify blocks that cannot be removed—the ones bearing the load of the stack—are said to be part of the structure’s “force chains,” the collection of pieces jammed together by the forces placed on them:

“We hypothesized that the ants could sense these force chains and avoided digging there,” Professor Andrade said. “We thought maybe they were tapping grains of soil, and that way they could assess the mechanical forces on them.”

A major challenge, however, was the need for a nondestructive method to characterize these structures as they were created. Another challenge was presented by the ants themselves.

With Caltech entomologist Professor Joe Parker, the team began culturing ants and learning how to work with them, which took nearly a year. Not only did they need to breed enough ants to work with, there was a lot of trial and error involved in getting the ants to dig in little cups of soil that they could load into an...
X-ray imager. Through that work, they determined an optimal size of cup to use, and an ideal number of ants to put in each cup. Still, the ants did not always cooperate with the researchers’ own priorities:

“They’re sort of capricious,” noted Professor Andrade. “They dig whenever they want to. We would put these ants in a container, and some would start digging right away, and they would make this amazing progress. But others, it would be hours and they wouldn’t dig at all. And some would dig for a while and then would stop and take a break.”

**ACTION**

In 2016, in collaboration with ARO Program Manager and Mathematics Branch Chief Dr. Joseph Myers, a workshop was organized on topics related to granular materials and mathematics. Professor Andrade participated in the workshop and conversations began on the intersection of his laboratory capabilities and pressing Army needs, especially as related to the modeling of vehicle–terrain interaction. DEVCOM GVSC is a leader in this type of modeling and participated in the workshop as well. Later in 2016, Dr. Barzyk performed a site visit to Professor Andrade’s laboratory at Caltech, during which they discussed the possibility to study excavation processes from a granular materials perspective. A proposal was submitted and accepted on this topic in 2017, and once the work was going, Dr. Barzyk encouraged the principal investigator to continue to follow Army developments related to vehicle–terrain interaction, which resulted in Professor Andrade participating in a weeklong demonstration event at a vehicle test course at the Keweenaw Research Center, Michigan, in 2018.

**RESULT**

Researchers X-rayed cups containing ants using a technique that created a 3D scan of all the tunnels inside (Figure 1). By taking a series of these scans, letting the ants work a little bit between each, the researchers could create simulations showing the progress the ants made as they extended their tunnels farther and farther below the surface.

Next, Professor Andrade’s team set about analyzing what the ants were actually doing as they worked, and a few patterns emerged. For one, Professor Andrade noted that the ants tried to be efficient as possible. That meant they dug their tunnels along the inside edges of the cups, because the cup itself would act as part of their tunnels’ structures, resulting in less work for them. They also dug their tunnels as straight as possible. Further, the ants dug their tunnels as steeply as they possibly could, right up to what’s known as the angle of repose. That angle represents the steepest angle that a granular material—a material made of individual grains—can be piled up before it collapses.

Through study of ant tunnels, the team discovered something that could one day be useful to humans: as ants remove grains of soil, they are subtly causing a rearrangement in the force chains around the tunnel (Figure 2). Those chains, somewhat randomized before the ants begin digging, rearrange themselves around the outside of the tunnel, sort of like a cocoon or liner. As they do so, two things happen: (1) the force chains strengthen the existing walls of the tunnel and (2) the force chains relieve pressure from the grains at end of the tunnel where the ants are working, making it easier for the ants to safely remove them.

Professor Parker calls this a behavioral algorithm:

“That algorithm does not exist within a single ant. It’s this emergent colony
behavior of all these workers acting like a superorganism. How that behavioral program is spread across the tiny brains of all these ants is a wonder of the natural world we have no explanation for.”

Professor Andrade says he hopes to begin working on an artificial intelligence approach that can emulate that behavioral algorithm so he can simulate how ants dig on a computer. Part of that emulation, he says, will be determining how to scale ant physics for human-sized tunnels.

WAY AHEAD

Professor Andrade is continuing this line of research as part of a Multidisciplinary University Research Initiative (MURI), co-managed by Dr. Myers in the ARO Mathematics Program, as part of a broader effort to determine how grain-scale features influence bulk materials properties. The modeling approach has been adapted to sea ice research in collaboration with the ERDC-Cold Regions Research and Engineering Laboratory.

In summer 2021, Professor Andrade’s Ph.D. student held an internship with DEVCOM GVSC in which he used modeling tools developed in this effort to enhance DEVCOM GVSC’s mobility simulation capabilities to include polydisperse particle sizes and arbitrarily shaped grains.

SUCCESS STORY

Urban Heat Islands during Heat Waves

The magnitudes of urban heat island (UHI) effects during heat waves (HWs) in two cities with contrasting climates (Boston, Massachusetts, and Phoenix, Arizona) were studied using the Weather Research and Forecasting (WRF) model. Significant differences were identified in heating and cooling effects during day and night between the two cities, indicating that the magnitude of UHIs and the associated effect of urban cool islands are strongly controlled by urban–rural differences in terms of aerodynamic features, vegetation and moisture conditions, and heat storage, which show contrasting characteristics in different regions. The research is described in a paper published in the Journal of Applied Meteorology and Climatology.

CHALLENGE

Despite having no universal definition, HWs usually refer to a sustained period (typically more than two days) when the temperatures (e.g., daily maximum, mean, or minimum temperatures) exceed a certain threshold. Recent years have witnessed numerous disastrous HWs worldwide, such as the 2003 HW in Europe, the 2010 Russian HW, and the 2013 HW in eastern China, incurring substantial socioeconomic costs and raising concerns about human health, wildfires, crop failures, and infrastructure damage. What is worse is that the intensity, duration, and frequency of HWs have been increasing and will likely continue to increase in many parts of the world in a warming climate. With the high thermal risks imposed by HWs in mind, the urban population, which comprises more than half of the world’s population and is projected to reach 68% by 2050, usually experiences hotter conditions than its rural counterpart due to well-known UHI effects. UHI effects have many impacts including to atmospheric boundary layer flow, the dispersion of pollutants, and energy and water consumption in cities.

Although the causes of UHIs are generally well understood, due to the difficulty or impossibility of making direct measurements of contributing phenomena, it remains a challenge to quantify their relative importance. These phenomena include lowered evapotranspiration associated with limited green space and low surface moisture, lower albedo owing to radiative trapping, and larger heat release at night due to the higher thermal admittance of built materials as well as larger anthropogenic emissions.

ACTION

This effort is one of a number the program has supported on the physical science of the built environment. Because of the expectation that the urban battlefield will become increasingly important as the global population continues to urbanize, it is critical that urban environments be characterized at a resolution that will enable environmental modeling, as well as maneuver and communication within them. Prior to being supported through the Earth Materials and Processes Program, very little basic research had been performed on this topic since the foundational work on UHIs in the 1970s. Beginning in 2015, Dr. Barzyk actively recruited a number of efforts with a focus on determining urban-surface properties and energy exchanges to enable high-resolution modeling and prediction in the built environment for Army applications. Professor Dan Li (of Boston University) is a
ARL Competencies:

Military Information Sciences

Mechanical Sciences

CHAPTER 3  
SUCCESS STORIES

CHAPTER 3  
SUCCESS STORIES

former student of program principal investigator Professor Elie Bou-Zeid at Princeton University, and Dr. Barzyk reached out to Professor Li soon after he began his position at Boston University to initiate discussions on Army-relevant potential research topics.

RESULT

The contributions of these processes to the magnitude of UHIs strongly depend on the nature of the urban and rural environments, human activities, and meteorological conditions. Moreover, the spatial variations of UHIs across cities and background climates and their key controlling factors are still under debate. To address this lack of knowledge, Professor Li and his team simulated the magnitude of UHIs during approximately 20 HW events from 2007-2016 over Boston, Massachusetts, and Phoenix, Arizona, using the WRF model and data from ground-based and satellite data (Figure 3). The objective of this study was to quantify and compare the underlying drivers of UHIs during HWs in the two cities with contrasting background climates (Boston having a humid continental climate and Phoenix having a hot desert climate). Conducting the same analyses over these two cities provided insights into the spatial variability of UHIs and their controlling factors.

Professor Li found that during the daytime, a surface temperature cooling in Boston occurred, mainly caused by the higher efficiency with which water is extracted from the ground to the surface or from within vegetation to the leaf surface, reducing latent heat flux, and due to higher urban aerodynamic resistance, which inhibits convective heat transfer between the urban surface and the lower atmosphere. In contrast, it was determined that daytime surface temperature in Phoenix is mainly controlled by the lower urban aerodynamic resistance, which facilitates convective heat transfer. At night, surface temperature and near-surface air temperature heating were identified in Boston due to the release of stored urban heat. In comparison, the lower urban aerodynamic resistance in Phoenix facilitates convective heat transfer from the atmosphere to the urban surface at night, leading to surface temperature heating but not to heating of near-surface air (Figure 4). This research indicates that the magnitude of UHIs is strongly controlled by urban–rural differences in terms of aerodynamic features, vegetation and moisture conditions, and heat storage, which show contrasting characteristics in different regions. Further investigation on the roles of anthropogenic heat flux, weather conditions, and further validation of the simulated results is recommended.

WAY AHEAD

The proposed effort is relevant to operations within the dense urban environment. Knowledge of the physical properties of the surfaces within the built environment is required to enable prediction dispersion of hazardous materials, air quality, extreme weather events, and the operation of unmanned aerial vehicles within an urban landscape.
SUCCESS STORY

Uncovering Nonlinear Flow Physics with Machine Learning and Sparse Modeling

When the equations that describe interesting phenomena become too complex (or worse, are unknown), it is still possible to learn new physics. Professor Steven Brunton at the University of Washington is building powerful new tools that allow the discovery of new models that are interpretable and generalizable.

CHALLENGE

For many systems of interest, the equations that govern their behavior are either complex or insufficiently well known. In addition, when the system dynamics is nonlinear (i.e., the relationship between variables cannot be described by the equation for a line) and high dimensional (i.e., the number of variables needed to describe the system become large), solving these equations often becomes intractable. Machine learning offers some enticing opportunities to contribute to these difficult problems, but often suffers from a general lack of interpretability (i.e., what is the relationship between inputs and outputs) and generalizability (i.e., will the results apply beyond the specific data used to build the model).

ACTION

In 2017, Professor Brunton sent a white paper to the Fluid Dynamics Program outlining ideas for using machine learning to design nonlinear control laws to better manipulate flows. During a telephone discussion of the details, Dr. Munson expressed concerns about the potential to gain fundamental knowledge of the flow physics, since many neural network approaches are unable to “look inside the black box” and say anything concrete about the “learned” input-output relationship. Dr. Munson suggested that perhaps another recently published result from Professor Brunton, known as sparse...
identification of nonlinear dynamics (SINDy), could be used to “peek inside the box,” thus interpreting the actions of the machine-learning control algorithm.

Roughly a week later, Professor Brunton emailed a new white paper combining machine-learning control (MLC) and sparse model identification to uncover and characterize new flow regimes and describe their underlying dynamics. Additionally, there is great potential to discover more appropriate basis functions through the use of genetic programming to provide an adaptive system identification process able to narrow in on the most appropriate sets of nonlinearities and nonlinear interactions for describing such systems. If ultimately successful, the framework may allow discovery of novel real-time adaptive sensorimotor flight control and the dynamics of a complex system such as a living organism. As Professor Brunton often observes at the beginning of conference presentations, biological systems provide “proof by existence” that management of complex unsteady flow fields is possible without knowledge of the governing equations and with only minimal computational expense.

RESULT

Professor Brunton’s efforts to date have been wildly successful, with notable contributions across a number of research areas.

One area involves discovery of models from data. The ability to do this task well has the potential to transform fields of science and engineering where large amounts of data are available but for which governing equations are unknown (or poorly known). Without a mathematical model, quantitative descriptions of behavior are difficult to generate and future behaviors are impossible to predict. While many approaches to constructing models are available, some recent advances in applied mathematics now permit the use of so-called sparse regression techniques to enable the determination of both the structure and parameters of a nonlinear system directly from data. Sparse regression techniques are powerful because they can often find the “simplest” equations required to describe the dynamics, attempting to balance the desire to have an accurate model that is also easily understood; the SINDy tool seeks to do exactly this (Figure 1). One of the important contributions from the current work has been the development of a means to discover not only the governing equations for the dynamics, but also the coordinate system in which those dynamics can evolve most compactly.

As a simple example, imagine a city with streets laid out on a north-south-east-west grid but having directions to a destination that use distances along NNW-ENE-SSE-WSW compass directions; in this case, the directions would be far simpler if everything was rotated by 22.5°. In the same way, finding a parsimonious representation for the dynamics involves having both the right coordinate system and an understandable governing equation in that frame.

Another area is the use of already known patterns to identify opportunities for sparsification. Many high-dimensional systems exhibit dominant coherent structures that evolve in a lower-dimensional space. These structures provide prime targets for the reduction of model complexity, since their dynamics can often be described with less effort than fully predicting behaviors across all scales. Several powerful methods have recently emerged for model reduction. In addition, recent advances in compressed sensing allow the use of a small subset of measurements to reconstruct a full signal. The amount of data is far below what is usually considered required by traditional techniques. Combining these two techniques offers the very real possibility to estimate and control systems with few measurements and sparse actuation.

With continuing advances in these two areas (discovering models from data and leveraging sparse measurements of that data), Professor Brunton and his team have made contributions across a wide swath of scientific fields. To date, the combined YIP/PECASE effort has resulted in 35+ journal publications with

Results

• Learned the governing equations and conservation laws from limited and noisy data.
• Derived mechanistic (not probabilistic) models of the dynamics of turbulent flows.
• Learned the dominant physical processes with data-driven balance models.

Anticipated Impact

Improved data-driven modeling and control of systems with complex dynamics (such as fluid flows) have the potential to significantly advance the performance of aerial vehicles, munitions and missiles, as well as distributed sensing and command and control applications.
This success was made possible by:

Dr. Matthew Munson, Mechanical Sciences Branch
Dr. Frederick Ferguson, Mechanical Sciences Branch (former)

Citations:


60+ coauthors. These papers have addressed not only the development of the tools and frameworks discussed previously, but have made contributions to understanding fluid dynamics, optics, magnetohydrodynamics, neurology, quantum systems control, wind energy, and more. Professor Brunton has also authored a textbook Data-Driven Science and Engineering (Figure 2) and has hours of companion lectures available on YouTube. The methods he and his team have developed are not only contributing to new discoveries in flow physics, but are fundamentally changing the nature of how scientific research is pursued.

WAY AHEAD

In addition to journal publications, Professor Brunton has presented his work in many forums, including to industry, at Army/DoD program reviews and workshops, as well as in focused engagements with DEVCOM ARL personnel. Projected to complete in FY23, Professor Brunton remains focused on developing a framework to control and characterize fluids that improves with increasing data, positioning it to capitalize on the big data revolution. Improved data-driven modeling and control of fluid flows has the potential to significantly advance numerous scientific, engineering, and industrial efforts, resulting in drag reduction, lift increase, mixing enhancement, and noise reduction.

SUCCESS STORY

Simple Ideas for Difficult Problems

CHALLENGE

While this challenge is well known and significant research is underway across the S&T enterprise to pursue various possible solutions, Dr. Hiroaki Nishikawa at the National Institute of Aerospace has taken a couple of particularly intriguing approaches. The first involves recasting the governing equations for fluid flows into a form that allows well-established numerical techniques to be applied. Techniques for solving equations in this alternate formulation are already established and well known to be efficient and accurate. The second approach involves exploiting concurrency, which involves finding ways to treat time as an additional dimension. This allows for the possibility to treat an unsteady flow in three dimensions (e.g., the flow over a helicopter rotor blade) as a steady flow in four dimensions.

The novelty of the first approach was recognized by a previous ARO Fluid Dynamics Program Manager Frederick Ferguson. He was interested in the potential to advance the ability to obtain efficient solutions to partial-differential equations (PDEs) numerically and started the first effort in 2012. When Dr. Munson took over management of the Fluid Dynamics Program in 2014, the effort had achieved reasonable successes in solving these reformulated equations. Dr. Munson funded a modification to the original effort to support the integration of the results (to be discussed in this Success Story) into NASA's fully unstructured Navier–Stokes solver (FUN3D). (Fully unstructured refers to the lack of regularity of the underlying grid on which the equations are solved. The Navier–Stokes equations are the governing equations for fluid flows for the majority of the aerospace applications typically encountered by Army vehicle and weapon systems).

Dr. Nishikawa’s continued ability to propose novel and innovative approaches to increase the accuracy and efficiency of CFD simulations and his dedication to using simple approaches to tackle difficult problems resulted in Dr. Munson’s continuous support for his research over two additional research proposals. Dr. Nishikawa’s currently supported effort leverages the results of earlier research to develop a highly accurate solver on adaptive space–time unstructured grids. Successful completion of this research can be expected to provide significant advances in CFD capabilities, simultaneously increasing efficiency and accuracy and establishing solid progress toward future 4D (space–time) simulations.

RESULT

Dr. Nishikawa’s early innovation has had an impact on solving a persistent problem in CFD: the accurate and efficient computation of gradients. Most CFD formulations solve some form of the Navier–Stokes equations and return the answer in terms of a velocity field; for each point in the simulated space, the speed and direction of the fluid flow at that point is calculated. While the velocity field is useful on its own, it is also important to know how fast the velocity is changing in some spatial direction (also referred to as the gradient). For instance, at a solid boundary, the gradient of the velocity is what allows the surface drag (skin friction) to be determined. Another flow feature that is calculated via a
Results

• Increased the speed and accuracy of CFD by changing the form of the equations to be solved.

• Exploited concurrency to solve an entire unsteady flow field in one step. If successes continue, these advances will eventually permit CFD tools to be significantly simplified, allowing such tools to be more robustly utilized for design of aerospace vehicles.

Anticipated Impact

Clever approaches to computing the solution of complex unsteady flows around Army aerial vehicles and weapons systems will lead to faster performance improvements in the design of such systems.
**SUCCESS STORY**

**Experimental and Numerical Investigation of the Deflagration of Energetic Materials at High Pressures**

Work supported by ARO led to the development of an ultra-high-pressure strand burner capable of reaching relevant pressures for the study of energetic material combustion to understand multiphase chemical and physical processes.

**CHALLENGE**

Current combustion models of many gun and rocket propellants do not well-predict burning rate as a function of pressure. The linear burning rate of a propellant or explosive is often described over a specific pressure range by the empirical equation \( r_b = aP^n \). The parameter \( a \) is often considered a function of temperature, while the exponent \( n \) is independent of temperature and describes the influence of pressure on the burning rate. Burning rate data of propellants and explosives have been measured for years using various experimental techniques such as photocinemicrographic and closed bomb combustion methods. In the photocinemicrographic method, the energetic material sample is pressurized in the combustion vessel, and a video of the sample regression is recorded for analysis of the burning rate. A small sample must be used such that the volume of gas produced from combustion does not contribute significantly to the overall volume of the chamber, allowing the assumption of constant pressure. The upper limit for these windowed chamber experiments has generally been about 50 MPa, although most are for 10 MPa and lower. For pressures higher than 50 MPa, the closed bomb technique is used in which the sample, in the form of a powder or strand, burns in a relatively small volume without observation. Pressure–time data are used to deduce the burning rate from a model developed to describe the experiment that must account for variable thermochemistry, heat losses, ignition, and flame spreading within the sample. The resultant empirical equation \( r_b = aP^n \) is valid for only limited pressure ranges. Composite propellants are also well known to exhibit slope breaks, burning rate plateaus, and even negative pressure dependencies. Most burning rate data are limited to...
pressures below 20 MPa, and for data greater than 50 MPa, observations of the burning processes are not available. The presence and behavior of non-ideal burning (burning in cracks, side burning, etc.) can therefore only be surmised. In addition, the manner in which burning rate changes with pressure when the temperature of the energetic material is varied (burning rate temperature sensitivity) can also change the dependence of burning rate on pressure. Understanding burning rate pressure and temperature sensitivity is key to propellant combustion response and stability. Finally, understanding the roles of real gas effects, supercritical behavior, soot formation, chemical mechanisms in the gas, liquid, and condensed phases, and a changing flame structure as a function of pressure is needed to allow for improved accuracy of future models.

**ACTION**

Dr. Anthenien has pushed the Propulsion and Energetics Program performers to conduct experiments at representative conditions since he took over the program in 2006. While experiments at atmospheric or moderate pressures can elucidate much in the way of burning behavior, at extreme pressures, three-body effects on kinetics as well as changes in phase behavior (supercritical pressures) can call into question assumptions about linear or even monotonic behaviors in pressure. Late in 2014, Professor Rich Yetter of Pennsylvania State University (Penn State) approached Dr. Anthenien about conducting high-pressure experiments using a yet-to-be-built ultra-high-pressure strand burner. In close coordination with Dr. Anthenien, Professor Yetter, in conjunction with Professor Mitch Smooke of Yale University, submitted a proposal in 2015 to the Propulsion and Energetics Program Single Investigator (SI) effort along with a proposal for a Defense University Research Instrumentation Program (DURIP) grant to build an ultra-high-pressure optical chamber for propellant and combustion studies. The objective of the SI effort is the development of a mathematical model for a three-tiered system consisting of solid, liquid, and gas to be developed in parallel with an experimental study of the combustion of energetic materials up to pressures of 300 MPa. The latter work was to be supported by high-pressure experiments in an optically accessible combustion chamber and strand burner proposed to be developed and built under the DURIP proposal. To allow time for the facility to be built, Dr. Anthenien delayed award of the SI effort until 2017 when the new ultra-high-pressure facility was ready for use.

**RESULT**

An ultra-high-pressure optically accessible combustion chamber was designed, developed, and implemented by Penn State researchers. The chamber has a 12-L internal free volume, providing enough room to house multiple different kinds of experimental modules. Additionally, the large free volume allows the reduction of pressure spikes during testing. The chamber is designed and rated for testing up to 300 MPa. To date, tests as high as 100 MPa have been conducted and already produced significant findings. Specifically, nitromethane and hydroxylammonium nitrate (HAN) burning rate data have been obtained for various pressures up to 100 MPa and various tube diameters ranging from 0.5 to 14 mm to deduce values in which turbulence and heat losses impact burning rate. To further investigate the roles of instabilities, turbulence, and transition to supercritical combustion on burning, liquid propellants were chosen that when burned would be dominated by condensed-phase reactions and by both condensed-phase and gas-phase reactions. The two systems chosen were an aqueous solution of HAN/water and HAN/water/methanol (Figure 1). For pressures below 30 MPa, the results indicated that HAN/water mixture burning rate was controlled by the condensed phase reaction where the rate was observed to be nearly independent of pressure except at the lowest pressures where the vaporization temperature of water was lower than the decomposition temperature of HAN. For pressures below approximately 7 MPa, the burning rate trends of the HAN/methanol/water mixture follow the same trends as the HAN/water burning rate. Eventually, the vaporization temperature of methanol increases above the HAN decomposition temperature of methanol increases above the HAN decomposition temperature of methanol.
temperature, and the methanol remains in the condensed phase, altering the reaction rate to slow the burning rate. The exact chemistry for this inhibition is not known but has been observed when other thickening gums have been added to HAN mixtures as well as nitrocellulose. As pressure is increased, the gas-phase reaction now contributes to increasing the burning rate. At 30 MPa, the HAN/water/methanol mixture burns as a cellular turbulent flame. Above 40 MPa, the flame goes dark, then a distinct interface reappears with some jetting from the surface, the visible turbulent flame structure disappears, and $r_b$ decreases by an order of magnitude. The burning rate as pressure is increased from 1 MPa to 70 MPa increases by a factor of ~15 up to about 10 MPa, then decreases back to approximately the same as that at 1 MPa. This latter unusual behavior may be related to the ionic nature of HAN and will be investigated in future studies. This study is the first of its kind to directly investigate propellant burning rates at these elevated pressures.

WAY AHEAD

Discussions with Army engineers at DEVCOM AC facilitated by Dr. Anthenien about using Penn State’s ultra-high-pressure chamber for testing of large-dimension gun propellant grains have resulted in a test program that is using the modular chamber to characterize the combustion behavior of large extruded propellant grains over a range of relevant pressure conditions for large-caliber gun systems under development by the Army. The combination of large internal volume and high pressure provided by the chamber built under ARO support is unique in the United States. The combustion data are to be made available to DEVCOM ARL researchers for modeling studies of propellants.

SUCCESS STORY

Vaporization, Mixing, and Ignition Dynamics in High-Pressure Evaporating and Reacting Sprays

Understanding spray development, including breakup and vaporization of the resultant droplets, for heavy hydrocarbon fuels at high pressure and temperature is key to understanding the ignition behavior. DEVCOM ARL–funded researchers developed and built a new high pressure and temperature spray vessel (HPTV) with optical access to allow use of laser diagnostics to characterize and measure developing fuel sprays under engine-relevant conditions.

CHALLENGE

Quantitative measurements of gas-phase fuel–air mixing are necessary to understand various combustion strategies and their effect on engine performance; however, the harsh environments of engine conditions make such measurements challenging. Previously, gas-phase mixing measurements in regions where liquid and gas phases coexist (“vaporization region”) have been difficult to conduct, and the data obtained had too large an uncertainty to provide significant value for model validation. Furthermore, detailed statistics of gas-phase quantities have not been available within the literature previously for regions with sizeable droplet concentrations. A key area of investigation in evaporating sprays is the spatial correlation between droplet concentration and gas-phase mixture fluctuations, including the effects of droplet clustering and segregation on liquid–gas correlation statistics. This information is critical for developing physically based models seeking to describe vaporization dynamics under high-pressure spray conditions.

ACTION

While there are a plethora of models for spray breakup, there is precious little validating data available. Dr. Anthenien has long engaged the optical diagnostic community to develop better methods for analyzing spray breakup and vaporization at high pressures and temperatures to provide validating data at engine-relevant conditions. Early in 2017, Dr. Anthenien coordinated with Professor Jeff Sutton of The Ohio State University to consider using the filtered Rayleigh scattering (FRS) technique in a pressurized optical chamber to allow spray characterization at relevant conditions. The significant advantage being that FRS allows for quantitative measurement of fuel vapor while in the presence of droplets. The information provided would also lend to better understanding of cool flame/low-temperature ignition phenomena and the postulated two-stage ignition that results.

RESULT

Professor Sutton developed and built a high pressure and temperature spray chamber to use FRS for quantitative fuel vapor measurements without interference from the surrounding droplet field. The researchers also used schlieren and simultaneous Mie scattering (liquid droplet phase) with the FRS
Results

• Used FRS in a high pressure and temperature spray chamber to obtain quantitative results of ignition height and delay times for a reacting spray.

Anticipated Impact

Deeper physical understanding of spray-breakup processes at pressure and improved models as a result of validation data.

ARL Competencies:

Mechanical Sciences

Figure 2: Comparison of liquid fuel penetration as a function of pressure (20 to 50 bar) for dodecane fuel.

measurements to investigate the two-way coupling between the dispersed liquid phase and the gas phase with a specific focus on how the two-phase interaction governs the fuel vapor–ambient mixing topology. In this way, a detailed statistical characterization of the liquid- and gas-phase structure can be performed, generating probability density functions and corresponding statistics of droplet loading, fuel vapor and temperature fluctuations, and the local mixing state (i.e., fuel-to-air ratio, equivalence ratio, mixture fraction). A systematic characterization of the HPTV to understand the fidelity of the test environment has been conducted, and the results show a thermally uniform test environment (maximum nonuniformity of 3%). This level of uniformity is ideal for interpreting ignition results and computational fluid dynamics model validation.

Measurements of fuel penetration as a function of pressure were also conducted. Figure 2 shows a set of image stills extracted from 50-kHz schlieren imaging showing a comparison of fuel penetration as a function of pressure. A diesel surrogate fuel was used, and the results show that with increasing pressure, fuel penetration is inhibited. There also is a buildup of liquid fuel at the leading edge of the fuel plume as pressure increases. The experimental data developed by these experiments will be critical for validating numerous spray-breakup models.

Theoretical development of the criteria for utilizing Abel tomographic inversion for statistically axisymmetric flows has also been accomplished. Many flow visualization approaches (i.e., schlieren) utilize path-integrated imaging. A long-standing question has been under what circumstances can the Abel inversion be applied and what statistics can be recovered reliably. The researchers have shown that for path-integrated data, only the statistical mean can be recovered, and higher-order moments cannot be reliably recovered as the statistical operator does not commute with path integration. Finally, the researchers conducted analysis on atmospheric ignition studies. During the HPTV construction, atmospheric ignition experiments were conducted to understand the most probable mixing, temperature, vorticity, and strain rates occurring at ignition. The experiments were only recently completed and all data has been analyzed; ignition height and delay times have been compiled and all image processing has been completed. The researchers are currently compiling the results and are expected to report/publish the results in the near future.

WAY AHEAD

High-speed Rayleigh scattering measurements will be conducted to determine the mixing field downstream of the liquid spray plume. Further, simultaneous OH* and Rayleigh scattering will be performed to correlate the most probable mixing conditions with the onset of high-temperature/second-stage ignition. Comparisons between the most probable mixture fraction facilitating ignition and the calculated most reactive mixture fraction will then be made. Additionally, high-pressure reacting spray studies, characterizing the statistics of ignition kernel formation location and timing and flame liftoff as a function of temperature, pressure, and liquid mass loading will be conducted. Professor Sutton is also currently collaborating with Dr. Campbell Carter at the Air Force Research Laboratory for investigation of their newly developed wavelet-based optical flow velocimetry for investigating cavity-stabilized scramjet flow paths. The current analysis shows velocity results with much higher spatial resolution compared to particle image velocimetry.
SUCCESS STORY

Predictive Modeling Framework for Nanocomposites for Ballistic Resistance

A mesoscale model has been created to study the fracture behavior of aligned neat cellulose nanocrystal (CNC) films, using atomistically informed coarse-grained models, and extended to describe material systems with other compositions and topologies. This model enables the prediction of the response and failure of a nanocomposite film at the mesoscopic scale of micro-ballistic experiments.

CHALLENGE

The properties of nanocomposites can be tailored on the mesoscale, offering a route to create materials with high ballistic resistance. Interfacial properties are known to play a critical role in the macroscale properties of nanocomposites; however, a fundamental understanding of the effects of the key properties of an interface, such as chemistry and structural orientation, on the ballistic performance of the materials is unknown.

ACTION

Program Managers at ARO began working with Professor Sinan Keten at Northwestern University to address this issue through a collaboration with DEVCOM ARL scientists who were studying nanoparticle interactions with polymers. In 2012, Professor Keten proposed a study to explain the role of CNC surface functionalization on interface and interphase characteristics of CNC neat films and nanocomposites using molecular and mesoscale theories and simulation techniques, and to corroborate interfacial characteristics with the macroscale mechanical behavior. The Solid Mechanics Program Manager realized that the model development aspects of this project would complement the work being performed at DEVCOM ARL and connected Professor Keten with Drs. Jim Synder and Jan Andzelm to collaborate on the project. During the course of the project, the Solid Mechanics Program Manager attended a 2016 ASME conference, where Professor Keten presented preliminary work on the simulation of ballistic impact on 2D materials, which sparked an idea for continued investigation. Subsequent discussions resulted in a proposal to investigate the size, microstructure, and surface chemistry–dependent mechanics of neat nanocellulose thin films from a molecular viewpoint, and to establish design principles for maximizing the performance of these nanostructured materials under micro-ballistic impact. Professor Keten continued to work with Drs. Synder and Andzelm on the new
ARL Competencies:

- Terminal Effects
- Weapons Sciences

**PROJECT:**

As Professor Keten continued to develop and extend his modeling framework, other DEVCOM ARL scientists and ARO Program Managers realized the predictive power of his simulation framework and potential to apply the methods to other material systems of interest. During a 2019 site visit to Northwestern University and follow-up phone conversations, Dr. Ford discussed potential extensions of the modeling framework to polymer grafted nanoparticle assemblies, and in 2020, Dr. Ford facilitated a collaboration between Professor Keten and Dr. Müge Fermen-Coker at DEVCOM ARL to extend the simulation framework to study the mechanics of atomically layered nanocomposite films under high-strain-rate deformation and impact conditions.

**RESULT**

A mesoscale modeling framework was developed to study the ballistic performance of nanocomposite materials using atomistically informed, coarse-grained molecular dynamics simulations. Figure 1 shows two examples of using this methodology to relate the ballistic performance of a film to its nanoscale features. In the first example (Figure 1a), Professor Keten studies a bioinspired system containing CNCs arranged in a Bouligand, or twisted plywood structure, similar to structures found in beetle exoskeletons and mantis shrimp dactyl clubs. The simulations reveal that an optimal pitch angle between the layers (18°-42°) leads to the highest ballistic resistance, significantly outperforming other pitch angles and quasi-isotropic baseline structures, which can be explained by improved energy dissipation through greater interfacial sliding, larger in-plane crack openings, and through-thickness twisting cracks. The second example (Figure 1b) shows the methodology applied to star-polymer–based thin films. The mechanical properties of the films were adjusted by varying the number and length of the arms in the polymer. The ballistic simulations revealed two components of the penetration energy: $E_{p,1}$, which corresponds to the early stage compression and correlates with the Young’s modulus and the Debye–Waller factor of the films; and $E_{p,2}$, which corresponds to late-stage backface deformation of the film and correlates with the films’ toughness.

**WAY AHEAD**

The results of Professor Keten’s recent studies are the beginning of the understanding of important chemical and topological factors that may be important for the design of nanocomposite systems for ballistic resistance. He is continuing to work with DEVCOM ARL collaborators to apply his simulation methodologies to study nanocomposite systems of interest to the Army.

**SUCCESS STORY**

**High-Strain-Rate Comminution of Granular Solids**

Continuum laws were formulated to explain the rate dependency of granular solids based on grain-scale dynamic processes, providing a means to quantify the dissipative capacity of these materials as a function of their grain-scale properties.

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**Figure 1:** (a) Bouligand microstructure of CNCs and the effect of pitch angle on the specific ballistic limit velocity ($V_{50}/r$) and energy absorption ($\Delta E_k/r$) in a thin film. (b) Star polymer topology and the effects of the mechanical properties of the films on the penetration energy. See Qin et al. (2019) and Giuntoli et al. (2021), respectively, for more details.
This success was made possible by:
Dr. Denise Ford,
Mechanical Sciences Branch

Citations:

ARL Competencies:

**Challenges**
Granular materials have excellent potential for energy dissipation and derive their unique properties from interactions between the grains and the propagation of these interactions across scales. Impact events in granular systems generate waves that propagate across the system and are weakened by local dissipation mechanisms. Comminution is an important mechanism of energy dissipation in granular solids where the particle size distribution is altered through surface area creation; however, an explicit link between the dynamics of comminution and its grain-scale origin was missing in continuum theories.

**Action**
Professor Giuseppe Buscarnera at Northwestern University first began to address this challenge through a Short-Term Innovative Research (STIR) grant in 2016 to explore the interplay between grain-scale energy loss through surface-area creation and the consumption of energy in granular systems undergoing simultaneous comminution, frictional shear, and volume change. This grant allowed Professor Buscarnera to obtain critical preliminary data that bridge fracture processes at the grain scale to the collective crushing of particle packings and formulate a new constitutive theory for granular continua, which captures the interplay between global dissipation and material microstructure. The results of this study were used as a basis for a follow-on Single Investigator (SI) award to explore the role of strain rate on the proportion of frictional and breakage dissipation in granular targets subjected to rapid loads, and to reinterpret their rate sensitivity in terms of the dynamics of crack growth at the grain scale. During the course of this new award, Dr. Ford encouraged Professor Buscarnera to use the Undergraduate Research Apprentice Program (URAP) to introduce an undergraduate student to Army-relevant research. Dr. Ford and Professor Buscarnera also participated in an Army Science Planning and Strategy Meeting on Controlling the Load Distribution, which sparked an idea for a future project that could build on some of the interesting results obtained from the SI grant. They are currently working toward the next steps to continue knowledge development in this area.

**Results**
- Developed new simulation tools to quantify the influence of grain-scale attributes rarely considered in continuum-scale engineering design protocols (e.g., particle size, shape, and polydispersity).

**Anticipated Impact**
An improved understanding of the mechanical behavior of granular media is expected to impact future designs of protective barriers in Army systems by diffusing shock waves from explosives.

**Figure 2:**
(a) Schematic of testing configurations aimed at determining the role of various factors on dynamic comminution. (b) Evolution of a 3D shape to the critical aspect ratio.

Professor Buscarnera conducted confined comminution experiments in packed granular samples, as shown schematically in Figure 2a, and developed a particle tracking algorithm to quantify the kinematics and morphology of individual grains. The experiments revealed that particle angularity promotes contact fracture and pervasive fragmentation. The experiments also revealed that the initial grain shape plays a key role during the first stages of loading leading to yielding, but its influence tends to vanish at high pressure, when cushioning mitigates the role of initial morphological differences and hinders further major breakage. Finally, the experiments revealed a correlation between the aspect ratio of the parent and child particles. A discrete element model was formulated to replicate the statistical variability of the particle strength and the multiplicity of the potential grain fracture mechanisms. The model can be used to simulate the comminution of crushable granular solids to study the response of granular solids at varying strain rates and to compute energy dissipation contributions at multiple length scales. Augmented breakage models were also formulated to capture multiple sources of dissipation in granular solids subjected to rapid loading. The models include a hypothesized critical aspect ratio that heavily crushed particles will converge to (depicted in Figure 2b), a particle shape–dependent strain energy potential, and a link between the particle shape and breakage growth rate. Finally, the models were implemented as user-defined models in the finite element code ABAQUS, a common engineering analysis software package, allowing one to quantify the influence of grain-scale attributes on breakage fields.

**Way Ahead**
Professor Buscarnera is continuing to study the evolution of particle shape during dynamic loading and plans to investigate the existence of the hypothesized critical aspect ratio, which is anticipated to further improve models for the mechanical performance of granular materials.
Dr. Bruce West

Dr. Bruce West served as the ARO Senior Scientist in Mathematics (ST). He received a B.A. cum laude in Physics from the State University of New York at Buffalo in 1965, and an M.S. (1967) and Ph.D. (1970) in Physics from the University of Rochester. Before coming to ARO as the Senior Scientist in Mathematics (ST), Dr. West was Director of the La Jolla Institute's Division of Applied Nonlinear Problems (1983-1989) and Professor of Physics (1989-1999) and Chair of the Department of Physics (1989-1993) at the University of North Texas (UNT). He was a founding member of the La Jolla Institute (1979) and Founding Director of the Center for Nonlinear Science at UNT (1994). Dr. West received the Meritorious Presidential Rank Award (2013) and the Distinguished Presidential Rank Award (2018), among numerous other academic and Army awards for research. He has authored over 300 peer-reviewed journal articles, 35 book chapters, and 21 books, receiving over 22.5K citations with an h-index of 73.

Retirement of Dr. Bruce J. West

Dr. Bruce J. West, ARO Senior Scientist in Mathematics (ST), retired in 2021 after more than 22 years of federal service (Figure 1). Across the Army, there are fewer than 30 senior research scientist positions, known as STs, who serve in general-officer level positions, advising leadership on science matters.

Dr. West has more than 50 years of experience in developing mathematical models to bridge the gaps separating the understanding and control of the complex phenomena within the life, physical, and social sciences. During his federal career, he developed and presented the mathematical basis for a new theory of medicine that led to revolutionary methods for mechanical ventilation, evaluating the treatment of depression and cardiopulmonary bypass pumps for critically ill and severely injured patients.

Dr. West also formulated a new mathematical strategy to facilitate overcoming the research barriers to critical Army problems imposed by complexity. With that effort, he changed the national university curriculum. It now includes a new kind of mathematics, fractional calculus, which is necessary for solving critical Army research problems in disciplines ranging from anatomy to zoology.

Dr. West’s work has quantified the information transfer between complex networks, as in the control of physiological systems by the brain, the adoption of an individual to social groups, and the control of crowds by zealots. He has authored more than 300 peer-reviewed journal articles, 35 book chapters, and 21 books covering an impressively large range of topics. His publications have garnered more than 23,000 citations with more than 600 for the year on the date of his retirement.

While at ARO, Dr. West also served as an adjunct professor at Duke University for almost 20 years. He plans to continue his research after retirement exploring threads of research including the inability of nonlinear equations to provide the kinds of forecasts made in efforts at predicting human impact on global climate change.

“Bruce’s professionalism, candor, his quick wit, and his desire to always add a different perspective to discussions about the future Army made DEVCOM ARL a better learning organization and truly set him apart as an advisor and a leader.”

Dr. Patrick Backer, Director DEVCOM ARL.

Figure 1: Dr. Patrick Baker (left), Director DEVCOM ARL, and Dr. Bruce J. West (right) at Dr. West’s retirement ceremony.
**SUCCESS STORY**

**Visual Search in Natural Images: Combining Brain Activity, Eye Movements, and Computational Models**

This ARO-funded research combined online behavioral studies, noninvasive neuroimaging techniques, eye movement recordings, and computational modeling to better understand visual search in a variety of contexts. The team studied how different tasks impact brain responses to eye fixations in natural scenes, developed a computational model that describes the sequence of fixations when searching for one target, and further implemented and validated a novel task to study foraging behavior (looking for more than one target) in natural scenes.

**CHALLENGE**

On the one hand, a major bottleneck in understanding the brain processes related to visual search comes from the fact that people normally move their eyes when looking for a target. The EEG sensors used to measure brain activity will also pick up these additional signals that are related to muscular movements. This project developed and improved a series of techniques that allowed better identification of brain activity. On the other hand, models of scene viewing that could successfully predict natural behavior should incorporate active interaction between perception and action, which poses a major challenge that Dr. Juan Kamienkowski’s team (Laboratório de Inteligência Artificial Aplicada [LIAA], Federal University of Paraíba) successfully addressed by encoding goals and guidance into a computational model.

**ACTION**

Dr. Anthony Ries’ program at DEVCOM ARL co-funded this effort. Periodic communication with the principal investigators brought to Ms. Szmigiel’s attention that to overcome difficulties in recent experimental science, research in the area must move forward with online experiments and computational models. As result, a collaboration with Professor Matias Ison from the University of Nottingham was recently established, which includes co-funding effort from the DEVCOM-Atlantic International Technology Center office. Professor Ison’s research effort includes collecting magnetoencephalography (MEG) data.

**RESULT**

The project contributed to three different areas.

First, in order to identify the modulation of stimulus processing by a task, an experiment was performed where participants saw a display (Figure 1A) and were instructed to search for a target (face or object) or freely explore the scene. EEG and eye movements were co-registered along with...
the task, preprocessed to clean for muscular artifacts, and compared using a deconvolution procedure. This procedure, based on linear regression, also enabled the team to explore other covariates of brain responses to individual stimuli. For instance, it was possible to consider the content of the fixated patch (face or object), which showed a characteristic N170 effect that resulted independent of the task, eye movements, or fixation rank in the sequence of eye movements. The task presented a fast response (~100-200 ms after the fixation onset) in occipital and frontal electrodes (Figure 1B).

Second, state-of-the-art saliency models have been useful to predict fixation locations in natural images, but provide no information about the sequence of fixations and are restricted to a raw observation task. Nowadays, one of the biggest challenges in the field is to go beyond saliency maps to predict a sequence of fixations related to a visual task, such as searching for a target. Bayesian observer models have been proposed for this task, as they represent visual search as an active sampling process. Nevertheless, such models were mostly evaluated on artificial images, and how they adapt to natural images remains largely unexplored. A Bayesian model for visual search guided by saliency maps as prior information has been proposed and validated with eye movements in a visual search experiment in natural scenes (Figure 2A). The resulting model performed very similarly to humans, with correctly identified targets found for a given number of fixations. More strikingly, the scan path, i.e., the entire sequence of fixations, results were indistinguishable from those of human observers (Figure 2B).

Third, while in a visual search, observers are required to memorize one potential target, there are real-life situations where more than one potential target could be present (hybrid search) and where items do not appear in isolation (Figure 3A). The team has recently shown that the main hallmarks of hybrid search remain present when contextual information is present and investigated how a variety of behavioral mechanisms, including working memory and inhibitory control, are active together in hybrid search (Figure 3B).

WAY AHEAD

The results of this collaborative research showed how using advanced deconvolution models can help to untangle different cognitive contributions to the process of visual search. A robust biomarker was found that could successfully separate visual search from exploration. Collecting a large dataset of participants performing a complex task that combines visual and memory search allowed the validation of previous laboratory results and further established that the main characteristics of this complex task are also present when the context is added to the images, which is closer to the real world. This work will bring together first and second initiatives mentioned. Moreover, future efforts will be made in extending the actual model to other search-related tasks including the hybrid search, thus adding third initiative mentioned to the scene.

Results

- Discovered new methods using advanced deconvolution models to process brain activity.
- Explored cognitive contributions to the process of visual search.

Anticipated Impact

Eye fixation-related neural activity may be utilized in future applications by enabling systems to interpret the relevance of information at each eye fixation while an operator searches a scene. Leveraging these neural metrics during visual search may enable intelligent systems to better predict a Soldier’s behavior and provide better adaptation during Soldier–system interaction.
Professor Kamienkowski worked with Professor Ison in securing follow-up funding from DEVCOM ARL to further expand this successful collaboration to incorporate MEG recordings, with their superior spatial resolution, as well as using dynamic stimuli (movies) to investigate neurophysiological markers of hazard detection.

SUCCESS STORY
Studies on the High Rate Behavior of Damaged and Granular Brittle Material

Funding from ARO is supporting an international and collaborative research program between Professor James Hogan at the University of Alberta, Canada, and DEVCOM ARL scientists on the design of next-generation ceramic-based materials used in armor applications. The program pushes the state of the art in experimental and computational materials science toward discovering behaviors that govern material performance. DEVCOM ARL is leading the transition of the data and predictive models to end-use.

CHALLENGE

The challenge in understanding the processes that govern the impact performance of ceramic-based materials used in advanced armor systems is that these processes evolve temporally and spatially over a very broad range of length (~nm to ~m) and time (~ns to ~ms) scales. At the nanometer and nanosecond scales, microstructure-governed mechanisms influence the very earliest stages of impact where decelerating the impactor is important. At the relatively larger meter and millisecond scales, structural deformation processes contribute to defeating the impactor. Throughout the impact process, failure mechanisms initiate, evolve, and compete with each other across these scales toward contributing to the overall system performance.

At the core of understanding these mechanisms are experimental and computational mechanics, whose fields have been driven by recent developments in new advanced diagnostics (e.g., laser-based probes coupled with field testing) and multiscale physics-based modeling approaches (e.g., mesh-free, phase-field approaches to accurately capture important failure mechanisms). These are overcoming previous barrier with technologies to capture experimental behavior, as well limitations in computational resources, to solve models efficiently and in reasonable amounts of time. Fundamentally, experimental and computational mechanics of materials research focus on understanding structure–property–performance relationships. The goal is to determine the length- and time-scale dependent failure mechanisms within materials for a given loading situation (e.g., ballistic impact). Once understood, we seek to improve material performance by controlling how they fail, and this is accomplished through materials design (e.g., ceramic-based composites) and fabrication using advanced technologies (e.g., 3D stereolithography printing).

To address these challenges and goals, multidisciplinary and collaborative partnerships are needed that can both make new discoveries through fundamental science, as well as accelerate the translation of this knowledge to end-use. This team makeup is the core to ongoing and long-lasting international collaboration among ARO, the International Technology Center – Americas, DEVCOM ARL, and the University of Alberta, Edmonton, Canada, and that collaboration underpins the success of this effort.

This success was made possible by:
Dr. Jonathan Ligda, DEVCOM ARL
Ms. Denisse Szmigiel, International Division

Citations:
SUCCESS STORIES

A RO began to support co-funded projects with DEVCOM ARL to support collaborations among Dr. Hogan and Drs. Tomoko Sano and Jonathan Ligda of DEVCOM ARL on understanding impact failure in ceramic-based materials and advancing strategies to design new materials that will better protect Soldiers. During this time, relationships were established and grown through exchanges, joint publications, and collaborative mentorship of graduate students working on the project. This collaboration has attracted participation of additional scientists over time (e.g., Drs. Matt Guziewski and John Clayton), and these relationships have led to 14 high-impact publications and 20+ conference presentations since 2016, as well as the organization of conference symposia (e.g., TMS 2020, Canadian Materials Science Conference 2018) and workshops (e.g., ARO-supported “Workshop on Mathematical Challenges in Brittle Material Failure” in May 2019).

RESULTS

Scientifically, the teams at the University of Alberta and DEVCOM ARL are making novel contributions in understanding the fundamental mechanisms that govern the performance of ceramic-based materials during impact. This is being accomplished through development and application of the most recent advances in multiscale experimental and computational mechanics approaches. Example highlights of the research outcomes from the program are shown in Figure 4. Here, the experimental and computational mechanics approaches used to study important length-scale dependent failure mechanisms that govern the impact performance of ceramic-based materials are identified. The goal of our program is to develop predictive models at the structural scale (to the right in the figure) that are informed and validated by subscale experiments and models. In turn, these predictive models are used to identify favorable material microstructures and mechanical properties that result in improved impact performance of ceramic-based materials.

Altogether, the research outcomes from this international collaboration are driving the state of the art in experimental and computational mechanics toward understanding the dynamic behavior of ceramic-based materials. These accomplishments of the program serve to attract promising and diverse graduate student researchers who provide innovative ideas to support and grow the program.

WAY AHEAD

Beginning in 2022, the team will begin work on new boron carbide-based composites in collaboration with Drs. Clayton, Guziewski, and Ligda of DEVCOM ARL. Scientifically, the research will focus on developing models that are faster, contain more physics across length scales, and can be more robustly validated with experiments; this will make the work more usable by U.S. Army engineers in the future. To address challenges with having faster models, they will explore the use of open-source platforms (e.g., FeniCS) that offer opportunities for highly parallelized and computationally efficient numerical algorithms that are more design-friendly. They will also leverage the latest in machine-learning based approaches to solve constitutive equations in micro-mechanical models, as well as develop new physics-guided atomistic potentials in molecular dynamics models. Validation will include comparing temporally and spatially resolved field measurements (e.g., temperature), and better evaluating and appreciating inherent variability and stochasticity in both experiments and models (e.g., real microstructures accounting for grain features). When completed, these higher-fidelity, multiscale models will provide new insights into the important mechanisms that govern performance of ceramic-based materials, and, in turn, can guide design of better-performing advanced materials with tailored microstructures and chemical compositions.

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Innovations in Materials Science International Program

Program Manager
Dr. James Harvey

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. He came to ARO in 1994 as the Program Manager for what was then called the Electromagnetics and RF Program after 21 years as a uniformed Army scientist.

CURRENT SCIENTIFIC OBJECTIVES

1. Leverage, for U.S. military research programs, novel and unique international research ideas and capabilities in the fields of materials science with a focus on the discovery of unique materials or materials composites or unexpected materials properties that, if successful, will provide new properties of materials for military application.

2. Develop new analytical and instrumentation capabilities to interrogate multi-dimensional evolution of materials structures, properties, and failure modes that, if successful, will enable the discovery and fabrication of new materials and composites with new properties or amenable to more efficient manufacturing.

SUCCESS STORY

Scalable Self-Assembly of Colloidal Crystalline Materials and their Inverses

Scientists at the University of Cambridge show that the dynamics of the self-assembly of a defect-free colloidal crystal depend primarily on shear and compressive vibrational forces, and that the key to attaining the maximum entropy (defect-free) state is to crystallize slowly.

CHALLENGE

Colloidal crystals form from particles substantially larger than atoms or molecules, and are arranged in a crystalline regular pattern (Figure 1A). The crystallinity results from the hierarchical arrangement, not necessarily from the constituents of the individual colloidal particles. The crystalline structure of mesoscale particles (larger than molecules, smaller than microscale) and sizes near optical, phonon, vibrational wavelengths provide properties significant for photonic, phononic, thermal, thermoelectric, and metamaterial applications. Opals are an example of this structure, formed by self-assembly naturally over millions of years. The inverse of the close packed structure of Figure 1A can be formed by injecting materials such as metals, polymers, ceramics, composites, and semiconductors into the interstices of the close packed structure and then dissolving away the colloidal particles, as shown in Figure 1B. The resulting regular porous framework is mechanically strong but very lightweight. It can be functionalized by the choice of intercalated material. In principle, the opal-like structure could be achieved by individually placing each colloidal particle from the “bottom up;” however, this process would not be capable of scaling up to a manufacturing process. Most efforts to grow films of colloidal crystals have resulted in highly defective morphologies. The primary barrier to the exploitation of these new opportunities for new functional materials structures is that the details of the self-assembly process of these close packed structures is poorly understood.

ACTION

Dr. Chakrapani Varanasi is chief of the ARO Materials Science Branch and Program Manager for Physical Properties of Materials, which has a focus on identifying new materials and material composites that have unusual properties amenable to exploitation for military application. Through scientific contacts and professional conferences, he realized the potential for new materials properties
using colloidal crystals and their inverses. In discussion with Dr. Bakas, Program Manager for Synthesis and Processing of Materials, they realized that the potential for these new materials complexes could not be realized without a credible path to large-scale fabrication. Professor Haydn Wadley, from the University of Virginia (UVA), had finished a project for Dr. Bakas’ program on fabrication of opal inverse materials. Professor Wadley had a long-standing collaboration with Professor Vikram Deshpande, University of Cambridge, who is a preeminent leader in modeling and theory of self-assembly of granular and colloidal materials. Dr. Bakas encouraged them to submit a joint collaborative proposal on a self-assembly process for colloidal crystals and inverses. Dr. Harvey, Program Manager for the ARO International Program in Innovations in Materials, co-funded the grant and provides in-country guidance to the Cambridge team and encouragement to emphasize collaboration with UVA. This grant is unusual in underlining the university-to-university collaborative channel as a conduit for transitioning international expertise to a U.S. university program, which is an active part of the U.S. Army’s research program and provides the transition path into the military programs.

**RESULT**

The team focused on a macroscale granular mechanics approach to understand the dynamics of the self-assembly of a defect-free close packed colloidal crystal under a compacting force. In this case, the compacting force is gravity, although one of the discoveries of the group is that such a constant can be modified or replaced by a magnetic force. The largely unsuccessful attempts by other groups resulted in a wide range of defects: stacking faults, vacancies, grain boundaries, dislocations, regions of non-close packed structure, voids, and crack-like flaws. The team focused on understanding the dynamics and control of the formation of these defects during self-assembly in order to develop an industrial-scale processing capability for thick materials suitable for engineering applications. From the largely unsuccessful previous attempts by other groups and simulations with their unique granular dynamics codes, the Cambridge team identified shear and compressive vibrational forces for research concentration. They have two unique capabilities for this research. The team developed powerful post-processing software to run in conjunction with the most recent granular mechanics models. And they have an X-ray computer tomography (X-CT) machine. Unlike most other labs, the Cambridge team is able to view the volumetric scans of the crystallizing structure in real time and by cross-sectional images.

As such, the Cambridge team was able to show that, counterintuitively, the ordered, crystalline configuration corresponds to the maximum entropy configuration. A key conclusion is that once a system has been disordered, it is difficult to order it completely. The answer to attaining the maximum entropy state is to crystallize slowly. A significant finding is that only a few particle and environmental capabilities for this research. The team developed powerful post-processing software to run in conjunction with the most recent granular mechanics models. And they have an X-ray computer tomography (X-CT) machine. Unlike most other labs, the Cambridge team is able to view the volumetric scans of the crystallizing structure in real time and by cross-sectional images.

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parameters determine the speed of crystallization. Stiffness, density, coefficient of restitution, and even particle size have little influence on the process rate. Vibrational frequency, amplitude of vibration, and strength of the gravitation force field collapse into a single significant parameter $\Gamma$, the vibration intensity, equal to $A \omega^2/g$, where $A$ is the amplitude of vibration, $\omega$ is the vibration frequency, and $g$ represents the acceleration due to the compacting force field (gravity in all the experimental results). A finding is that theoretically $g$ can be altered by a magnetic field, which is important for manufacturing process development. The force of inter-particle friction also has an important effect. Horizontal vibration (or vibration perpendicular to the compacting force) is found to be more effective for crystallization than vertical vibration. The reason is that vertical vibration disrupts the order in the crystallizing lower layers, while horizontal vibration provides enough energy to overcome barriers to particle rearrangement.

The crystallinity fraction results from different process parameters (stiffness, density, coefficient of restitution, gravity force, vibration amplitude, and vibration frequency) (Figure 2), but the only parameters with an effect on the crystallinity fraction are vibration amplitude, vibration frequency, and gravity (the compacting force perpendicular to the vibration direction). Figure 2A clearly shows the collapse of these three parameters into a single parameter, $\Gamma$. (The results shown in Figure 2A are simulated.) Figure 2B shows the good comparison of simulation and experiment over the reduced range of $\Gamma$. Higher values of $\Gamma$ cannot be reached with the current experimental apparatus. Higher $\Gamma$ values will be explored in the next year’s research plan with a newly designed vibration system. The Cambridge team has identified the underlying physics of these curves. As the kinetic energy transferred to the colloidal particles increases (to the left side of Figure 2A), the particles are better able to overcome the barriers of movement along the surface until all of the particles have sufficient kinetic energy and the curve “saturates” (mid part of the figure). As the vibration frequency increases further, the kinetic energy transfer tends to be isolated near the boundaries of the colloidal collection leaving the center without sufficient energy to overcome barriers. Figure 3 shows that friction also has a significant effect on crystallization of the colloidal structure.

The principal investigator, Professor Deshpande, received a number of honors and awards resulting in part from his research on this project, including the Gili Agostinelli Prize for pure or applied mechanics.
or classical mathematical physics awarded by Accademia della Scienze, Torino, Italy (2021) and the Distinguished Alumnus Award, Indian Institute of Technology, Bombay (IITB) (2021). He was named a Fellow of the Royal Society of London (2020) (the Science Academy of UK, British Commonwealth including Australia, New Zealand, Canada, South Africa, Singapore, and India); no more than 48 Fellows are elected every year across all physical, biological, and mathematical sciences. He also received the Rodney Hill Prize in Solid Mechanics (2020), which is awarded once every four years by the International Union of Theoretical and Applied Mechanics to a single researcher, and was also named Fellow, Institute of Materials, Minerals, and Mining (2020).

WAY AHEAD

The Cambridge team is providing real-time updates to the UVA team on their discovery of processing parameters, which UVA is using to design a Bridgeman crystal growth production apparatus (Figure 4) to demonstrate industrial scalability as part of the ARO Synthesis and Processing of Materials Program. The results will be in the ARO extramural program in universities and a resource for military-related programs as well as industrial development programs exploiting the unique characteristics of this new material form.

During the next year of the project, the team will address the self-assembly of colloidal crystals from a liquid solution and the high vibration intensity behavior of the self-assembly process. The right-hand side of Figure 2A, which shows the fall off of crystallinity as $\Gamma$ is increased beyond about 8, is based on simulation only. The experimental validation in Figure 2B only goes up to a $\Gamma$ of 5. The Cambridge team has designed a unique vibrational shaking apparatus capable of high-amplitude horizontal vibration at high frequencies (high $\Gamma$). This work is critical to verifying that the high $\Gamma$ region is understood.
Computational Architecture and Visualization Program

**Program Manager**

Dr. J. Michael Coyle

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 came to ARO in 1999 as the Program Manager for what was then called the Discrete Mathematics and Computer Science Program (now Computational Architectures and Visualization).

**CURRENT SCIENTIFIC OBJECTIVES**

1. 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 that, if successful, are anticipated to lead to enhanced training capabilities for more effective combat readiness.

2. Create new energy-efficient techniques and architectures for the optimal realization of multicore systems, as well as future hybrid and exascale systems, to process and operate in resource-constrained environments that, if successful, will support complex, resource-demanding, real-time battlefield applications.

3. Devise scalable and communication-efficient algorithms to effectively handle the volume, heterogeneity, and multimodality of complex data arising from emerging and future Army applications that, if successful, will provide real-time, accurate delivery and analysis of critical Army data to all necessary and relevant combat units.

**SUCCESS STORY**

**Visualization of Discontinuous Galerkin-Based High-Order Methods**

This ARO initiative resulted in the design and implementation of a new visualization technique for high-order scientific computations significantly reducing the visualization error at a reduced computational cost. This new technique will potentially allow Army computational scientists to view results without loss of accuracy due to the visualization technique.

**CHALLENGE**

High-order finite element methods (FEMs) have reached a level of sophistication that allows them to be commonly applied to a diverse set of real-life engineering problems. Many of the physical problems of interest are, unfortunately, not steady-state, leading to simulations that must run for a long time. Thus, data-sets can easily consume all available storage and networking resources. Examples of such simulations within fluid dynamics include all simulations in which the fluid is in transition or fully turbulent. With regard to Army interests, problems in turbo-machinery and rotorcraft, where aspects of the geometry are rotating and/or sliding past one another, fall into this category. High-order FEMs are now beginning to be used to simulate these physical systems due to their inherent ability to capture complex structures, such as vortices (vorticity is a derived quantity from the velocity field indicating how fast the fluid is spinning), with little numerical dissipation and dispersion. The transient nature of these simulations complicates the data handling (postprocessing requires the time history) and renders single snapshots of the solution insufficient to understand the time-varying nature of the physics.

There is now a growing acceptance in the simulation and visualization communities that co-processing (in situ processing) is the most effective and least intrusive way to understand the results from transient simulations. However, if not done properly, a visualization system can introduce its...
Results

• Published three journal articles describing the design of a new visualization method for scientific computing.

• Incorporated new methods into an open-source visualization code.

Anticipated Impact

The Army scientific computing community will potentially benefit from this effort by significantly enhancing their ability to accurately and efficiently render simulation results, allowing for increased understanding of the underlying physics they are attempting to model.
the characteristic length that adaptively scales the L-SIAC filter across different resolutions of an unstructured computational mesh. This adaptive characteristic length produces a lower error on the nonuniform unstructured mesh and generates a smaller, if not the same, error on uniform meshes. They also showed that their algorithm is computationally efficient in high-resolution regions of the mesh and is computationally faster than using maximum edge length over the entire mesh. Professor Kirby’s team has applied this technique to both 2D and 3D fluid flow problems. Figures 1 and 2 show the results for a 2D simulation of flow past a cylinder.

**WAY AHEAD**

Future work needs to include the anisotropy of the mesh as an input to the algorithm to help estimate the best direction(s) and scaling for the L-SIAC filter. It is anticipated that Army scientists from DEVCOM AvMC and the DEVCOM ARL Visualization Lab will provide guidance in this process and be the ultimate transition partners. It is also planned to extend the method to utilize multiple CPUs and GPUs to gain further speed-up.

**SUCCESS STORY**

**Interactive Visualization System to Analyze Network Behaviors**

This ARO initiative resulted in the design and implementation of a new visualization technique for analyzing network traffic and detecting abnormal behavior. This new technique will potentially allow Army network security personnel to more efficiently detect security risks to Army networks.

**CHALLENGE**

The protection of computing infrastructures is an essential consideration in network security. Numerous studies have been proposed to monitor and detect suspicious or intrusive network activities. To protect Army computing infrastructures and confidential data from network intruders or attacks, designing innovative approaches (including visual analysis techniques) to identify intrusive network activities is considered one of the highest-priority research topics in network security. Conventional techniques for intrusion detection systems (IDSs), including host-based ID and network-based ID, identify threats by comparing incoming network activities to known attack patterns (i.e., signatures). While these techniques accurately discover known attacks, they are largely incapable of detecting unknown attacks. It is still a major challenge to identify unknown security threats since attack patterns are diverse and continuously change over time. Changes in network traffic patterns with newly emerged computing technologies make it even more difficult to detect the attacks accurately. Many existing intrusion detection techniques perform an event-based analysis that analyzes each network event independently. However, attackers initiate multiple consecutive network events (i.e., attacks) to intrude computing networks or systems. Analyzing network traffic data to detect suspicious network activities (i.e., intrusions) requires tremendous effort due to the variability of the data and constant changes in network traffic patterns. Therefore, existing techniques may not be suitable for analyzing sequential network events. It is also difficult to understand attackers’ temporal behaviors (i.e., behavioral changes over time), which compounds this challenge.

**ACTION**

Dr. Coyle was approached by Professor Soo-Yeon Ji, a researcher from Bowie State University who was interested in support regarding her efforts in developing visualization techniques to aid in the analysis of network behavior, especially in regards to network security. This is an area of great interest to the Army and DoD, so Dr. Coyle felt support was highly warranted and provided guidance for a proposal submission. This proposal led to the researcher being selected for an Research and Education Program (REP) award in this area. After the award was in place, Dr. Coyle conducted a site visit at Bowie State University to meet Professor Ji in person, review her progress, and see what aid could be offered in terms of connecting her with interested Army scientists. During this site visit, the Dr. Ji expressed a desire to be a summer visiting scientist at DEVCOM ARL’s Adelphi location. Dr. Coyle explained

This success was made possible by:

Dr. Charles Kamhoua, DEVCOM ARL Network Security Branch

Dr. J. Michael Coyle, Computing Sciences Branch

Citations:


“Since protecting computing infrastructures is a priority concern in business industries, understanding network patterns quickly and accurately is a critical step for detecting abnormal network activities.”

the timeline and process to the researcher, and an application was submitted. However, due to COVID-19, this opportunity was never realized. Fortunately, though, as a result of the application process, a connection was made with a DEVCOM ARL computer scientist in the Network Security Branch and a collaboration was established. This collaboration has resulted in a number of useful and applicable techniques, conference presentations, journal articles, and an invention disclosure submission.

RESULT

Understanding network activities has become the most significant task in network security due to the rapid growth of the Internet and mobile device usage. To protect Army computing infrastructures and personal data from network intruders or attacks, identifying abnormal activities is critical. Extracting features from network traffic data is considered an essential task to be performed because it affects the overall performances to identify the activities accurately. Although researchers proposed several approaches, they mainly focused on identifying the best possible technique to detect abnormal network activities. Only a few studies considered using feature extraction techniques. The researcher at Bowie State University teamed up with a DEVCOM ARL computer scientist and developed a new approach, with which an integrative information feature set is determined to identify abnormal network activities using wavelet transformation. Instead of extracting features by attributes, the approach uses all attributes' information to extract features and to design a reliable learning model to detect abnormal activities by reducing false positives. Two machine learning techniques, Logistic Regression (LR) and Naive Bayes, were utilized to show the effectiveness of the approach (Table 1). A visualization method was also devised and used as an aid in the analysis (Figure 3). As a result, they found that their approach produces a better performance result with less computational time in detecting abnormal network activities.

WAY AHEAD

In the future, it is planned to test and extend this approach on different, more varied, and larger network traffic data-sets at different time scales to estimate the attack risk of each event over time. It is anticipated that the collaboration with computer scientists from DEVCOM ARL’s Network Security Branch will continue, that they will provide guidance in this process, and will be the ultimate transition partners.

<table>
<thead>
<tr>
<th>Raw features</th>
<th>Wavelet features</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>LR</td>
</tr>
<tr>
<td>Accuracy</td>
<td>91.8%</td>
</tr>
<tr>
<td>False Positive</td>
<td>8.3%</td>
</tr>
<tr>
<td>Precision</td>
<td>91.9%</td>
</tr>
<tr>
<td>Recall</td>
<td>91.8%</td>
</tr>
</tbody>
</table>

Table 1: A performance comparison with two classifications (LR and Naive Bayes).

Results

- Established a collaborative effort with DEVCOM ARL’s Computational and Information Sciences Directorate.

- Published two IEEE conference papers, submitted two journal papers that are under review, and submitted an invention disclosure application.

Anticipated Impact

Designing a secure, stable detection technique to identify and respond to malicious cyber threats in a timely fashion is crucial. Developing a monitoring system to predict suspicious attacks and showing them with visual representation has the potential of significantly enhancing the understanding of attack activities directed toward Army systems.
Dr. MaryAnne Fields

Dr. Fields completed her undergraduate studies at the University of Louisville, receiving her B.S. in Mathematics in 1980. She continued her studies in applied mathematics at Clemson University, receiving her Ph.D. in Mathematics in 1988.

She came to ARO in 2019 as the Program Manager for what was then called the Intelligent Systems Program.

SUCCESS STORY

Human-Guided Unified Learning of Tractable Probabilistic Models

This ARO initiative has led to a principled approach to incorporating domain knowledge and human expertise into deep neural networks (DNNs) using intuitive logic-based encodings similar to IF-THEN rules. This approach reduces the training data required and allows subject-matter experts to guide the DNN training process without requiring them to be experts at machine learning.

CHALLENGE

DNNs have been successfully adopted in several applications—these models have produced impressive results in object recognition, natural language processing, and language translation. However, achieving these impressive results requires significant computational power and gigabytes of correctly labeled examples involving relatively simple data types (vectors, tensors, matrices, etc.). Designing applications for the real world will require researchers to address open challenges such as learning with sparse and noisy data (some of which are incorrectly labeled), generalizing to new settings, and working with relational data that describe multiple objects and their relationships. Humans often solve these learning dilemmas by incorporating knowledge from domain experts. Injecting domain knowledge into neural networks is an area of active research with questions such as where should knowledge be injected in the network? How can the contribution of external knowledge be measured? How can knowledge be propagated through the network?
Chapter 3: Success Stories

Results

- Developed a new framework for K-CLNs that provides a mechanism to incorporate external knowledge into column networks using intuitive logic-based encodings similar to IF-THEN rules.

- Determined that a K-CLN provides an efficient and effective learning strategy that exploits external knowledge to learn in environments with sparse and noisy samples.

Anticipated Impact

The K-CLN enables humans to guide the learning during the training phase of a DNN by providing preferences, or conditional rules, which improves the efficiency and effectiveness of current neural network training methods. This could have a significant impact on several future Army systems that utilize artificial intelligence/machine learning components, to include vehicles such as the Next Generation Combat Vehicle and Future Vertical Lift systems.
natural disaster. The K-CLNs converged faster, as shown in Figure 2, reducing the number of training samples required to train the model. He evaluated the robustness of the model by injecting noise in the human advice and varying the tradeoff hyperparameter, alpha, discussed previously. High values of alpha led to deteriorated performance, since it overvalues faulty advice from the human experts. The experiments showed that for alpha in the range 0.2–0.4, the performance of K-CLN is equivalent to the original CLN networks, despite the faulty advice. K-CLNs provide a promising approach to combining expert knowledge with neural networks in domains with multiple objects and multiple interactions among those objects.

**WAY AHEAD**

This research is part of a larger effort to develop unified, efficient, effective, human-guided algorithms for learning TDPMs. This project will first develop formalisms for unifying different data types, domains types, and model types. Effective learning methods for both discriminative and generative TDPMs based on gradient-boosting will be developed. Finally, these algorithms will be extended to handle rich human guidance in the form of qualitative constraints and preferences.

Long-duration autonomy requires intelligent systems to manage information from different sources, including humans, knowledge bases, and external and onboard sensors. This work will provide a foundation to managing different types of knowledge from multiple sources. Professor Natarajan’s research could impact ongoing Army efforts to develop robust and reliable autonomous systems that can connect multiple sources of information to better understand the environment, leading to better decisions in areas such as navigation, maneuver, and threat analysis. Dr. Fields is working with the Artificial Intelligence for Maneuver and Mobility Essential Research Program (AIMM ERP) to find ways to incorporate this work into their efforts to develop autonomous navigation and maneuver. Professor Natarajan’s research may enable these systems to develop a deeper understanding of the environment around the vehicle, which could impact its maneuver decisions.

**SUCCESS STORY**

A Deep Reinforcement Learning–Based Long-Term Tracker for Salient Event Detection

ARO-funded research has improved long-term visual object tracking (VOT) in complex environments by developing a novel approach to scale estimation that uses a computationally efficient, filter-based approach that considers both the peak filter response and its fluctuation to increase the confidence in the object localization.

**CHALLENGE**

VOT is the problem of continuously localizing a target in a video sequence given a single example of its appearance. While it has been studied for a number of years, there are still a number of challenges that prevent robust and reliable tracking of objects over extended time periods in complex environments. As a target moves through the environment, issues like motion blur from either target or camera motion make it difficult to maintain a track on a given target. Parts of the environment may be similar to the object, offering camouflage and making detection difficult. Illumination changes such as shadowing and glare change the appearance of the object, forcing algorithms to rely on the geometric properties of the target. However, deformations of non-rigid bodies reduce the reliability of these geometric properties. Large-scale variations resulting from movement along the camera’s axis are difficult for existing tracking methods to accommodate in complex image sequences. Real-time tracking also presents challenges—methods to reacquire targets should meet the strict constraints of time and computational budget, especially with respect to mobile operating systems or embedded computing architectures.
ACTION

Dr. Fields recognized that long-term object tracking in complex environments is a fundamental skill for future robotic systems that integrates sensing, reasoning, and efficient computation. As described previously, even when the target is visible, it can undergo significant changes in scale, aspect ratio, or illumination that make tracking challenging. Complex environments, like urban settings, contain buildings and other features that temporarily occlude a target, requiring systems to quickly reacquire targets. However, targets can be intelligent, so systems must reason about the actions of those agents to understand where and when to reacquire the track. For some future systems, like small unmanned aircraft, the processing needs to occur in near real time using constrained computational resources. These issues are starting to be addressed by the VOT community, which offers a yearly challenge (since 2018) to spur the development of long-term trackers. Dr. Fields recruited Professor Scott Acton of the University of Virginia’s Image and Video Analysis Laboratory to extend his work in tracking.

RESULTS

VOT is a fundamental task in image and video processing. This work addresses two challenges in long-term VOT: (1) compensating for large variations in the target scale resulting from movement along the camera’s axis in complex image sequences and (2) real-time tracking that meets the strict constraints of time and computational budget, especially with respect to mobile operating systems or embedded computing architectures.

VOT methods are generally divided into two types, generative and discriminative. Generative tracking methods learn a model to represent the appearance of a target object in one frame, and then the tracking problem is formulated as finding the most similar object in future frames. However, it can be difficult to model an object without considering background information when the background is cluttered or the target object is occluded by some other object. Most state-of-the-art VOT approaches are discriminative tracking methods. These approaches try to learn a model of the tracked object by treating instances of the background as negative samples and instances of the target object as positive samples. Among these methods, discriminative correlation filter (DCF)–based methods yield both high accuracy and high efficiency. Most DCF-based trackers employ a fixed size template and performance degrades when scale variation is encountered. This research addresses tracking problems with large scale variations in complex environments.

Standard DCF methods learn a correlation filter that depends on inexpensive image features rather than a deep learning approach. During learning, these methods approximate a dense sampling scheme by generating a circulant matrix, of which each row denotes a circular shift of the base sample. In such a case, the regression model can be computed in the Fourier domain, which brings significant speed improvement in both training and testing processes. During testing, most DCF methods use a simple criterion, the maximum response value, to obtain the best scale estimation.

In contrast, Professor Acton’s group incorporates a novel criterion called the average peak-to-correlation energy (APCE) that uses both the peak value and the fluctuation of the response map to find the best candidates for target location. Their method, Scale Invariant Tracking using Average Peak-to-Correlation Energy (SITUP), demonstrates a 2.7–5.2% improvement in the precision score over other discriminative trackers.

As an additional benefit, the robustness of the APCE criterion provides a significant performance gain for the tracking algorithm. In DCF methods, the computational costs are dominated by the fast Fourier transforms (FFTs) used to compute the correlation filter during the learning process. The number of required FFTs scales linearly with respect to the number of features used in the filter. Professor Acton’s team was able to use principal component analysis to significantly reduce the number of features. In experiments on the OTB benchmark datasets, Professor Acton’s algorithm demonstrated superior performance in both accuracy and speed.

WAY AHEAD

This work is part of an overall effort to address the long-term tracking problem in which the target object may undergo significant appearance changes. Tracking and detection cannot solve the long-term tracking task independently. Professor Acton’s approach tackles this problem by decomposing long-term tracking into three subtasks: short-term tracking, learning, and detection.
Dr. Hamid 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. at Northeastern University. He joined ARO in 2019 as the Program Manager of the Information Processing and Fusion Program.

SUCCESS STORY
Query-Based Data Acquisition for Target Detection and Estimation

A theory for query-driven target sensing was developed. It aims at constructing methodologies for understanding a scene or for recognizing a target in the presence of limited communication or a noisy channel through collaborative and/or human-in-the-loop sensing, which is particularly important and timely for human–machine teaming and other prospectively resilient autonomy.

CHALLENGE

The Army’s diverse tasks of interest often result in complex data in a contested or adversarial environment. Performing in a rapidly varying, noisy, and possibly hostile environment with limited transmission channel capacity or power/energy highlights the difficulty of a given mission. The challenge of obtaining a principled and systematic sensing strategy is real, and additional mitigating recourse is sought using a query-driven sensing system, which focuses the inquiry and appropriately enhances the retrieved information.

ACTION

Multi-Domain Operations entail multimodal sensing and often face adversarial environments that limit the objective performance. Recognizing this problem, Dr. Krim engaged the research community at large—including Professor Alfred Hero at the University of Michigan.
and DEVCOM ARL researcher—to pursue a "strategic" sensing that would include an ordered "sense and adapt" mechanism. This strategy may be viewed as an augmented sensing capability. However, its inspiration can be ascribed to a coaching/therapist role often found in training for helping to improve an individual’s performance.

RESULTS

A collaborative sensing strategy using a query-based mechanism was developed. An example of this mechanism would be a commanding officer generating queries for a Soldier in the battlefield who in turn follows through with a sense-and-respond provision. A sample query-driven target search is shown in Figure 1. It entails a 20-question target probing combined with an estimation mechanism that progressively and sequentially adapts in response to overcome any prevailing obstacles. Virtual, remote sensing is carried out by a query-based strategy (Figure 2) to overcome a constrained environment, keeping the agent away. Resolution limits for such a strategy are achieved and optimally established.

WAY AHEAD

The promise of this research was quickly recognized by Dr. Krim, who subsequently developed a collaborative research effort that led to joint publications (Chung et al., 2017; Zhou et al., 2021). The relevance to the autonomy-related core competencies (Military Information Systems and Network, Cyber, and Computational Sciences) is one pathway to potential integration and easy transition. For example, a tool on a personal device may be envisioned as a query-driven decision aid.

SUCCESS STORY

Sample Efficient Learning at Deployment Time

Autonomy is reliant on inference, which, in turn, hinges on learning at a cost of large training datasets. This work succeeds in minimizing supervision data at deployment time in typically DoD data-starved environments, thus making machine learning viable for the battlefield.

CHALLENGE

The influence and power of so-called deep learning has the potential to weaken the current state of autonomy. This is on account of its sample complexity and inability to generalize to novel classes and concept drifts or adapt to unanticipated/unscripted tasks and adversarial attacks.

ACTION

Autonomy inherently hinges on a machine’s capability to classify and recognize the environment and its contents and adapt to its changes. While recognizing that artificial intelligence has registered

Figure 2: Generic collaborative and information-driven sensing with query-driven adaptive sensing (courtesy of T. Coleman).

Figure 3: Low-complexity model representation and geometric constrained attributes.
significant progress over the last decade, limitations persist with the required training/sample complexity and sometimes prohibitive demands for diversity. This as a result, impacts its broad adoption and delivery of the promises for Army modernization priorities. To help mitigate these shortcomings and account for Army’s missions goals, Dr. Krim has engaged the research community. Through indepth discussions, these issues were viewed in a new light and a new potential avenue of research was suggested. The principal investigator, Professor Venkatesh Saligrama of Boston University, has offered a unique perspective regarding humans’ natural initial parsing approach of objects for recognition and understanding.

**RESULT**

The proposed inference paradigm is motivated by the natural human instinct of parsing objects of interest into easily interpretable concepts whose composition provides a meaningful summary. Specifically, salient functional representatives of an object (an image, for example) and their prominence captured by characteristics with associated semantic tenor and their corresponding parameters such as position within the object, together with their geometrically constrained structure, are learned, as illustrated in Figure 3. So describing an object effectively yields a low complexity/dimensional representation that achieves an exceedingly efficient approach to obtaining templates for inference and can adapt at deployment with very low sample complexity. These learned and reusable templates from prior episodic experiences and their characteristic geometry at the locations (illustrated in Figure 4), as well as their composition rules, result in a powerful and robust inference framework.

The few-shot-recognition algorithm is based on evaluating five-way one-shot and five-way five-shot accuracies (i.e., five classes are randomly selected from the test set, and one or five samples are drawn from these classes as support examples). This evaluation demonstrates the relatively efficient learning at deployment, with the results shown in Table 1.

The comparison was carried out with the state of the art, and the average accuracy is shown in Table 2.

**WAY AHEAD**

This promising work is being developed; collaborations with researchers from Army research laboratories should simplify the transition of evolving developments.

<table>
<thead>
<tr>
<th>Methods</th>
<th>One-shot</th>
<th>Five-shot</th>
</tr>
</thead>
<tbody>
<tr>
<td>FEAT</td>
<td>66.78</td>
<td>82.05</td>
</tr>
<tr>
<td>DeepEMD</td>
<td>65.91</td>
<td>82.41</td>
</tr>
<tr>
<td>TRAML</td>
<td>67.10</td>
<td>79.54</td>
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<tr>
<td>DPGN</td>
<td>67.77</td>
<td>84.60</td>
</tr>
<tr>
<td>Simple CNAPS</td>
<td>77.40</td>
<td>90.30</td>
</tr>
<tr>
<td>Ours</td>
<td>76.42</td>
<td>91.50</td>
</tr>
</tbody>
</table>

Table 1: Few shot learning results on recognition using the Stanford car as an object.

<table>
<thead>
<tr>
<th>Methods</th>
<th>One-shot</th>
<th>Five-shot</th>
</tr>
</thead>
<tbody>
<tr>
<td>ProtoNet</td>
<td>61.47</td>
<td>75.72</td>
</tr>
<tr>
<td>MetaOptNet</td>
<td>56.36</td>
<td>67.57</td>
</tr>
<tr>
<td>DN4</td>
<td>70.32</td>
<td>85.16</td>
</tr>
<tr>
<td>Ours</td>
<td>81.41</td>
<td>92.87</td>
</tr>
</tbody>
</table>

Table 2: Average accuracy comparison.

**Figure 4:** An object example captured by a geometric constraint between wheels and door window features.
CHAPTER 3  
SUCCESS STORIES

KNOWLEDGE SYSTEMS PROGRAM

Program Manager
Dr. Purush Iyer
Chief, Computing Sciences Branch

Dr. Iyer completed his undergraduate studies at the 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, after leaving his tenured, professor position at North Carolina State University, and has built up programs in various aspects of artificial intelligence (AI) and in network science. He currently runs the Knowledge Systems Program.

CURRENT SCIENTIFIC OBJECTIVES

1| Develop human-level communication that is key for adoption of autonomous systems by large swaths of society that address issues within human communication (being structured but highly contextual) that are needed to advance natural language processing, in particular methods that employ deep learning for processing that, if successful, will enable human–robot interaction as well make autonomous systems human-like in their interaction.

2| Advance algorithms that scale well in size yet retain their ability to look for human interaction, in the form of graphs and sub-graphs, be it the presence of adversaries in small groups within a large population or patterns of theft in financial transactions and other important questions that need to be answered to deal with both internal and external threats that, if successful, will impact social network analysis and how we deal with threats from adversarial groups in a way that is less computationally expensive.

SUCCESS STORY

Higher-Order Geometry and Topology of Complex Networks

By using simplicial complexes (SCs) (Figure 1)—a generalization of graphs—as the mechanism to capture non- dyadic (mainly group) interaction in social networks, Professor Ali Jadbabaie at the Massachusetts Institute of Technology (MIT) and his colleagues Professors Austin Benson and Jon Kleinberg at Cornell University have advanced a precise mathematical formulation of several social phenomena, such as homophily and weak ties, which social scientists understood but could never define, thus, solving an open problem in the literature. SCs were thought of as being too unwieldy for algorithmic development, but the team has shown that complexity can be tamed by building on the famous PageRank algorithm.

CHALLENGE

Graphs are inadequate to describe human interactions and, in particular, groups that occur naturally in social networks. Furthermore, hypergraphs and SCs are potential representations for groups. However, generalization of the traditional algorithms, such as PageRank or random walk, on graphs has been eluding the community.

ACTION

Complex networks underpin every area of current and future military and civilian infrastructure systems as well as integral parts of the biological, physical, technological, and socio-economic universe. Thus far, such networks have been mainly represented and analyzed as graphs, and tools from graph theory are commonly used to analyze such systems. However, while graphs can capture pairwise interactions between nodes, fundamental interactions in networks often take place among multiple nodes for which hypergraphs and SCs are more appropriate models. Given this scientific challenge and after seeing researchers working under the DEVCOM ARL Network Science Collaborative Technology Alliance fail to generalize social network analysis algorithms and, thus, abandon research in SCs, Dr. Iyer reasoned that (1) generalization of algorithms to hypergraphs could depend on domain knowledge and (2) that

This success was made possible by:
Dr. Purush Iyer,
Computing Sciences Branch

Citations:

Results

• Reinigrated old sociological processes by providing new mathematical tools to analyze how communities form and how the strength of ties affect information flow by accounting for both dyadic and group interactions explicitly.

• Featured in Quanta Magazine (https://www.quantamagazine.org/how-big-data-carried-graph-theory-into-new-dimensions-20210819/), which discussed how these researchers are turning to the mathematics of higher-order interactions to better model the complex connections within their data.

Anticipated Impact

Scalable and precise social network analysis to find communities (adversarial groups) and influencers in a society are important problems in military intelligence.

Result

Professors Benson, Jadababaie, and Kleinberg have laid the foundation for breathing sociological meaning into higher-order structures such as hypergraphs and SCs. The study has led to a mathematical explanation of sociological phenomena like homophily (the tendency of people with similar interests to form groups). Working on that foundation, they have devised a completely new definition of the notion of weak ties, which provide avenues for maximum transfer of information in a social network. Existing approaches, based on graphs, define tie strength based on the number of shared neighbors between individuals, or equivalently, the number of triangles in the graph that contain a specific pair of individuals. However, this approach misses out on critical information because it does not distinguish the case where interactions occur among groups involving more than two individuals. A new measure, called Edge PageRank, explicitly accounts for higher-order interactions in the network. Indeed, they show that Edge PageRank can be interpreted as the steady-state outcome of a dynamic, message-passing social process that characterizes the strength of weak ties by appropriately discounting the effect of higher-order interactions involving three individuals. The resulting algorithms have been validated against several large datasets. This the first time, since the seminal work of Granovetter in the 1970s, that we now have a formal mathematical approach for identifying weak ties in networks. This work will be submitted to the Proceedings of the National Academy of Sciences.

Way Ahead

This research team plans to expand upon the theory and techniques developed so far to detect mesoscale structures in higher-order data and massive social datasets. With the foundation laid, the DEVCOM ARL researchers who were originally interested in SCs will reengage and (potentially) collaborate with the MIT–Cornell group. Algorithms, as well as knowledge, will be tested out in the Network Science Research Laboratory for use in social network analysis.

Success Story

Adversarial Machine Learning Using Sparsified Front Ends

A method to protect deep neural networks (DNNs) that have been trained on valid inputs has been designed based on sparse coding inputs. With the new front end, researchers at the University of California, Santa Barbara have been able to show that the combined networks are immune against several common classes of attacks.
CHALLENGE

Machine learning (ML), especially DNNs, has garnered a lot of press due to advances in systems that play chess, Go, and other games effectively. However, ML-based systems can be brittle when faced with perturbed inputs (sent maliciously by adversaries), and there are many examples of how deep learning is susceptible to perturbations to the input, especially in the vision domain, which cannot be perceived by the human eye. While existing efforts to solve this problem have been top down, the approach followed here is bottom up with attention paid to the design of the networks.

ACTION

The Army is faced with many difficult issues, both on and off the battlefield, that many experts feel ML techniques have the potential to overcome. However, the scientific challenge, coupled with a lack of interpretability of DNNs, is a major impediment to the use of DNNs in safety-critical applications such as vehicular autonomy. In response, Dr. Iyer sought out proposals that characterize how DNNs operate and use that characterization to weed out input, or ameliorate the effects of adversarial input, without losing the inference power of the trained network. After considering a number of potential researchers and varied approaches, Dr. Iyer recruited Professor Upamanyu Madhow of the University of California, Santa Barbara. Dr. Madhow is a world-renowned researcher and expert in wireless communications, information theory, and information forensics and security.

Professor Madhow’s research involved understanding DNNs in order to make them more robust. This would be accomplished by imposing sparsity constraints to attenuate and eliminate adversarial perturbations with the goal of obtaining interpretable designs with guaranteed resilience. This is in contrast to state-of-the-art defenses against adversarial perturbations, which are based on black box training with adversarial perturbed examples. Deep learning techniques are being deployed aggressively by industry, given their spectacular performance improvements over classical approaches in many fields. However, for the Army to harness these techniques on the battlefield for situational awareness or intelligence gathering, where they can lead to life-or-death decisions, it is essential that these techniques come with robustness guarantees. In addition, these techniques need to be interpretable, so that decisions based on them can be better informed. This fundamental research is taking the first steps toward both of these objectives.

RESULT

The original hypothesis was that exploiting the sparsity of natural data would attenuate adversarial attacks, but design and experimentation have shown that (1) sparse projections alone are not enough and (2) it is essential to utilize nonlinearities and stochasticity. Professor Madhow and his team have shown that introducing drastic nonlinearities, together with a learned basis that suitably shapes the input, yields robustness comparable to the state of the art (purely black box training with adversarial examples). Initial results with this approach were validated with the simpler Modified National Institute of Standards and Technology database (MNIST) and Fashion-MNIST datasets and published as a conference paper (at the International Conference on Acoustics, Speech, and Signal Processing). For more complex datasets such as the Canadian Institute For Advanced Research (CIFAR)-10, the team developed learned, over-complete representations, which together with drastic nonlinearities, sparsity, and randomization, yield performance comparable to state-of-the-art defenses. The team was also able to provide a statistical analysis of the impact of adversarial perturbations and expended substantial effort designing attacks targeting their defense, since standard attacks were less effective. Because of the randomization in their encoder (Figure 2), the attacker needs to expend significantly more computational resources than what is needed to attack state-of-the-art defenses based on adversarial training. This work has been submitted to the Conference on Neural Information Processing Systems.

WAY AHEAD

The investigator will be using the new architecture for fingerprinting wireless transmitters as part of a Defense Advanced Research Projects Agency program. Furthermore, the bottom-up approach will need to be combined with traditional approaches, especially in the context of systems containing multiple learning-enabled components. It is anticipated that DEVCOM ARL’s Network Security Branch will provide guidance in this process and will be the ultimate transition partners.

\[\text{Figure 2: Neuro-inspired autoencoder.}\]

This success was made possible by:

Dr. Purush Iyer, Computing Sciences Branch

Citations:


Results

• Demonstrated that DNNs are easily fooled by perturbations in input.

• Showed that preprocessing input, much like type-checking in programming, can be used to filter out bad inputs.

Anticipated Impact

This research could lead to one of many necessary techniques to build robust AI-based systems.
SUCCESS STORY

Predicting Tissue Dynamics Based on Variations in Cell Stiffness and Clustering

This ARO initiative resulted in a novel algorithm to compute cell-to-cell interaction, and individual and collective migration in 3D complex environments that allows for long-term prediction of a cell’s trajectory. Beyond understanding key mechanistic drivers of health and disease in tissues and organs, the predictive models developed here will be extremely useful in improving regenerative therapies where engineered 3D environments are used to regrow and mend injured tissues. The migration of native cells into implanted 3D scaffolds and the growth and colonization of these environments are critical aspects of regenerative medicine, an area of high interest for the U.S. Army.

CHALLENGE

Cell migration and active rearrangements within the tissue environment are critical to a variety of biological processes such as tissue regeneration, wound healing, and cancer progression and metastasis. Variations in the properties identifying individuals within a given population are the norm in biology. This concept holds true at various hierarchical levels in biology, all the way down to the individual cells that make up the tissues and organs of the body; each cell is slightly different in its biochemical and biomechanical properties from the other cells that make up the tissue. This heterogeneity is the effect of the stochastic nature of biological processes that result in the properties of cells. An important question then arises, if the extent of variations observed within a given population is known, can that information be used to predict the long-term dynamics of that particular population?
Dr. Pasour initially met with Professor Parang Katira at San Diego State University (SDSU) to discuss Professor Katira’s ideas for studying the effect of heterogeneity in the biomechanical properties of cells and how their spatial and temporal arrangement could be indicative of the growth of cancerous tumors. Dr. Pasour immediately recognized its promise toward understanding the processes involved in tissue regeneration and wound healing, a critical area of research for Soldier care. Also, changes in the biomechanical properties of white blood cells were recently shown to be an early indicator of sepsis. As Dr. Pasour’s program already included a primary thrust area in the Fundamental Laws of Biology and, in particular, the issue of the function of heterogeneity/stochasticity had recently arisen at an ARO-supported workshop as an important question across many biological disciplines, she quickly recognized the potential contribution of Professor Katira’s research to her program and encouraged him to submit a proposal. Five months later, in September 2017, the ARO Biomathematics Program was able to begin supporting this research. This was the first major extramural funding for the lab and provided support for the training of one doctoral student in the Joint Doctoral Program between SDSU (a minority serving institution) and the University of California, San Diego (UCSD; a top R1 university in bioengineering). The grant also supported research training for two SDSU undergraduate student researchers in Professor Katira’s lab during the summer semesters. Dr. Pasour is currently working with Professor Katira on a new Single Investigator (SI) proposal that will leverage the previous research to further understand factors that drive self-segregation and spatial clustering of cells in dense tissue environments (packing fraction ~1).

Figure 1: Weakly adherent cells (a) have increased contractility (c) and higher stiffness (d) compared to strongly adherent cells (b) as determined based on detachment under shear flow. The mechanotype controls migration and durotactic behavior (e), and is dependent on actin-myosin activity (f).

Professor Katira’s team developed a novel algorithm to compute cell-to-cell and cell-to-matrix interactions in 3D heterogeneous, fibrous environments that allows the simulation of individual and collective cell migration occurring over days within minutes as a function of various cellular and extra-cellular mechanical properties. This allows for an accurate prediction of a cell’s path persistence and speed as it migrates through a 3D environment over several hours to days. Using this model, they show that depending on cellular mechanical properties and intercellular interactions, distinct strategies exist to maximize collective cell migration in heterogeneous environments. This new model also helped Professor Katira obtain preliminary results for two successful National Science Foundation (NSF) proposals, one in collaboration with UCSD and another with the University of California, Los Angeles (UCLA). In further collaboration with UCSD, they studied how heterogeneity in cell adhesion strength allowed a subpopulation of cells to ignore mechanical signals present within the tissue environment and migrate independently of stiffness gradients, while most other cells migrated up the stiffness gradient (Figures 1a-1e). This aberrant behavior of a subpopulation of cells is directly governed by the differences in their mechanical properties (Figure 1f). These results were described in a paper published in the journal Cell Reports in 2021. Combining cell motility and differences in cell proliferation induced by heterogeneous mechanical interactions between neighboring cells, Professor Katira’s team was also able to explain anomalous mixing and de-mixing behavior of two different cell types observed in-vitro, results that were published in the New Journal of Physics in 2021. Building on the success of these theoretical models, they have further ventured to understand how spatial biomechanical heterogeneity in a cell population influences overall population dynamics. Their latest results show that the ratio of local to global heterogeneity in a tissue environment, a measure similar to “patchiness” used by ecologists, can be used to predict long-term changes in the tissue environment and the growth and dominance of particular subpopulations of cells.

**Anticipated Impact**

The results from this project shed new light on the role of cell-level heterogeneity in biomechanical properties, a process central to wound healing and wound closure. Additionally, models of cell proliferation and death as a function of cell mechanical interactions provides new insight into tissue regeneration, aging, and cancer progression.
WAY AHEAD

The ARO award has helped Professor Katira establish strong experimental collaborations with labs at UCSD and UCLA, and obtain additional funding to support these collaborative projects from the NSF. These projects go deeper into the molecular factors that dictate cellular biomechanical properties (collaboration with UCLA) and cell–environment interactions (collaboration with UCSD). While Professor Katira’s models can predict cell behavior and tissue dynamics based on differences in individual cellular mechanical properties, and cell-to-cell and cell-to-environment interactions, through the course of the project, additional factors that influence overall tissue dynamics have come to light that need further investigation. The first one is the emergence of multicellular phenomena, where collective cell behavior transcends individual cell interactions, for example, the formation of continuous mechanical structures that span multiple cells or the flocking of certain cells together giving rise to flow patterns during migration. Understanding how this higher order emerges in dense cellular constructs, such as tissues, and how it drives self-organization and pattern formation are the focus of a new SI proposal to be submitted by Professor Katira. The second area of interest that needs to be investigated is the coupling between the cell cytoskeleton and cell nucleus. In their current models, Professor Katira has assumed that cellular mechanical properties are directly coupled with cell nuclear mechanical properties. While this assumption is largely supported by literature, there have been recent studies that show, in certain scenarios, this coupling between the nucleus and the cell cytoskeleton can be tenuous and the mechanical properties of one might differently influence cell behavior than the mechanical properties of the other. Professor Katira’s lab is already working on developing models that integrate the cell nucleus and its links to the cytoskeleton within the models for individual cells.

SUCCESS STORY

Collective Behavior Emerging in a Heterogeneous Cell Population

This ARO initiative resulted in the development of a novel approach to the analysis of complex, irregular distributions of biological cells or other elements forming complex geometric structures. This approach integrates state-of-the-art machine-learning techniques with a new algorithm for representing arbitrarily complex geometric shapes with a mathematical graph. Such a method provides a highly efficient and precise tool for automated extraction and quantification of imaging information. It was successfully applied for the dissection of the intertwined regulatory processes driving the development of cerebral cavernous malformation (CCM), a disease that leads to hemorrhagic stroke but has no cure to date. However, this methodology is very broadly applicable and will serve the biomedical research community well beyond the specific applications of the funded project.

CHALLENGE

Studying physiological processes in health and disease is fundamentally difficult due to the broad range of temporal and spatial scales of the interactions involved in such processes. Indeed, knowing a mutation responsible for the onset of a disease does not immediately suggest a cure. To develop pharmacological treatments, scientists need to understand how the deficiencies at the molecular level translate into cell malfunctioning and, ultimately, into organ failure. Despite its many successes, the field of cell modeling is still limited to narrowly focused studies that oversimplify the problem, sometimes ad absurdum (to the absurd). Professor Denis Tsygankov’s lab at the Georgia Institute of Technology (Georgia Tech) is taking advantage of the increasing power of computational resources to develop new types of comprehensive models that bridge multiple processes across different scales, and thus form an indispensable part of the progress toward understanding deficiencies at the molecular level and their ramifications at the cell and organ level.

ACTION

Before becoming an Assistant Professor at Georgia Tech, Tsygankov worked as a postdoctoral fellow in the laboratory of Professor Timothy Elston at the University of North Carolina on a project funded by an ARO award under Dr. Pasour’s management. As a part of a site visit in 2015, Dr. Pasour had a meeting with Tsygankov, where he presented his ideas for extending the cell dynamics studies in the lab to a new direction that would allow efficient analysis of the collective cell behavior. Dr. Pasour’s program already included a thrust area in Multiscale Modeling/Inverse Problems and she quickly recognized the potential contribution and impact of comprehensive modeling across multiple scales of the physiological cellular processes proposed by Tsygankov and encouraged him to pursue this direction. A year later, as a new faculty member, Professor Tsygankov collected preliminary results and...
proposed a SI research project to the ARO Biomathematics Program that was funded in 2017. This support made possible the involvement of graduate and undergraduate students in the research project, which relied on the close integration of experimental studies with mathematical modeling and new methods of data analysis, and was the first major extramural funding source for the laboratory.

**RESULT**

The cell model developed in the Tsygankov lab explicitly accounts for protrusive activity, cytoskeletal stiffness, and forces developed through cell interactions. These features allowed the team to achieve exceptionally accurate quantitative correspondence between the simulated and experimentally observed dynamics at the single- and multicell levels. The model was applied to dissect biomechanical contributions to the collective behavior of endothelial cells under diseased conditions and in response to pharmacological treatment. The results of this work were published in *iScience* (Cell Press) in 2018. The team also developed an algorithm that can extract a comprehensive set of geometric measures from imaging data with arbitrarily complex cell shapes and multicomponent structures (Figure 2). By integrating this information-rich shape representation with a novel machine-learning algorithm, the team was able to analyze, with exceptional accuracy, multicellular patterns with subtle structural variations. The paper reporting this three-year effort was published in *PLoS Computational Biology* in 2020.

In parallel, the Tsygankov lab developed a new method that may change the way researchers perform ratiometric analysis of fluorescence resonance energy transfer biosensor data at the cell edge. The Noise Correction Factor method suppresses noise-related artifacts, thus allowing precise measurements of the signal in cell areas that would otherwise be excluded from the analysis. This advance led to an intriguing discovery that a protein Asef, which is involved in the activation of the key regulators of cell motion, GTPases Rac1 and Cdc42, concentrates in two distinct locations of cell protrusions where it behaves drastically differently over time. Identifying and characterizing such spatiotemporal segregations of protein activity are critically important for unveiling molecular mechanisms governing cell dynamics. The manuscript on this topic was published in *Frontiers in Cell and Developmental Biology* in August 2021. Following on these developments, in September 2021, a paper in *Scientific Reports* presented a model that reproduces a complex self-organization phenomenon in starfish oocytes, in which Rho GTPases activity partitions into multiple coexisting regions of coherent wave propagation, so-called wave domains. The model not only reproduced the cell-level activity of this key cytoskeletal regulator with numerical accuracy (as measured by textural characteristics of the spatiotemporal patterns), but also led to a number of intriguing discoveries. For instance, it revealed that the development of the wave domains is preceded by a phase of low activity, which may not be readily observed in experiments but has distinct characteristics that define the actin dynamics at the later stages of cell regulation. An automated tool of wave domain detection developed in the lab revealed an unexpectedly sharp reversal of pattern formation in the middle of anaphase in starfish oocytes. These discoveries illustrate that the new hybrid approach, which integrates reaction-diffusion models with biomechanical representations of moving and interacting cells being developed in the Tsygankov lab as a part of the ARO project opens new avenues for the mechanistic understanding of highly complex physiological processes across multiple scales.

**WAY AHEAD**

During the award period, the major focus was on the development of novel enabling methodologies in modeling and data analysis. A number of important discoveries were made as a part of the validation process for the developed tools. For example, the team discovered that despite significantly increased bundling of actin filaments in all three variants of CCM (CCM1, CCM2, CCM3), only CCM1 and CCM2 types have the expected increase in the overall cell stiffness as compared to healthy cells. This result is important from the pharmacological treatment perspective. Many other potential applications exist for the new hybrid approach. Thus, the immediate plan of the Tsygankov lab is to disseminate its software tools, models, and analysis methods to the broadest audience; establish new collaborations; and help other researchers to take advantage of these technologies. See, as an example, his prior work on CellGeo (*IEEE Trans. Med. Imaging* 38, 862-872 [2019]).

**RESULTS**

- Developed a biomechanical cell model that allows an in-depth understanding of the effects of drug treatments on collective endothelial behavior, which can be used to characterize the efficiency and potential side effects of these treatments in the context of angiogenesis, fibroplasia, and tissue regeneration—processes that are essential to wound healing.

**Anticipated Impact**

Combining this quantitative, predictive model with the new algorithm for the analysis of complex cellular patterns makes possible an integrative approach that is expected to lead to significant advancements in the fields of brain damage, such as that resulting from traumatic injury or hemorrhagic stroke, which might lead to improvements in stroke prevention and post-injury rehabilitation care of U.S. Army veterans.
SUCCESS STORY

New Computational Methods for World-Class Engineering Modeling in Army Turbine Applications

Investigations and investments in new types of mathematical operators are developing a best-in-the-world capability for high-fidelity fluid-structure interaction design and wear-resistance, as found in DEVCOM ARL’s turbine applications and others.

CHALLENGE

To a large extent, much of engineering design is built on the tools of calculus, and the mathematical operators of calculus are generally the tools that help describe and model the processes of convection, diffusion, radiation, continuity, and others. Problems arise when trying to account for unobserved/unmeasured processes, such as appear in or give rise to mixing, anomalous diffusion, surface ablation, wear, and others. The preceding processes share the property of being described by local operators—that is to say, each process is described more accurately by considering decreasingly small domains and seeking high fidelity in the limit as each domain of interaction shrinks to zero. Yet these models often do a poor job of describing observations of the process; one should be wary of any model that needs to include anomalous anything in order to describe observations. So the objectives of this effort are to (1) identify mathematical constructs that are not based on local operators, but rather admit nonlocality in order to analyze processes, and use these as the basis for new models; (2) develop computational methods for solving these new types of equations; and (3) demonstrate the validity of the methods in the context of an application that is important to the Army.
ACTION

The first step along this path was for Dr. Myers to help suggest and sponsor an invited conference in this area; this conference was held in Newport, Rhode Island, in 2015 and attracted mathematicians from across the United States and Europe. Based on presentations there and follow-on discussions, Dr. Myers and Dr. Matthew Munson, Fluid Dynamics Program Manager, teamed up to author a Multidisciplinary University Research Initiative (MURI) topic in the area; the winning team was headed by Brown University (Professor George Karniadakis) and included Michigan State University, Columbia University, the University of South Carolina, and Rice University. The project, "Fractional PDEs for Conservation Laws and Beyond: Theory, Numerics and Applications," focused on developing nonlocal operators, which by definition allow both action at a distance and (causal) memory effects. After the first couple of reviews, Dr. Myers arranged for the annual reviews to be conducted at DEVCOM ARL with Dr. Anindya Ghoshal’s group. Dr. Myers arranged all future reviews to be held there (first in person and later virtually). The academic team was able to share advances with lab personnel and, after a couple of years of work and initial successes, share with the government team their newly developed solver for Physics-Inspired Neural Networks (PINNs).

RESULT

One of the challenges involved in solving fractional-order partial differential equations (PDEs) is in applying correct and consistent conditions at the boundaries; unlike integer-order PDEs where the number of boundary conditions is just the operator order, there is a continuum of conditions to potentially be applied. The principal investigators have been able to develop this computational method, PINNs, to determine the fractional operator order based solely on boundary data, requiring no other derivative data (Figure 1). This works by approximating the unknown solution as well as the nonlinear dynamics by two deep neural networks. The first network acts as a prior on the unknown solution and essentially enables avoiding numerical differentiations that are inherently ill conditioned and unstable. The second network represents the nonlinear dynamics and helps distill the mechanisms that govern the evolution of a given spatiotemporal dataset. This is a significant advance; it greatly simplifies numerical solutions of these fractional-order PDEs with more accuracy and reduced runtime.

ARL Competencies:

Network, Cyber, and Computational Sciences

Results

• Developed a new computational method, PINNs, that greatly simplifies numerical solutions of fractional-order PDEs in engineering contexts with significantly increased accuracy, which is expected to lead to new design tools in a variety of engineering applications.

Anticipated Impact

Development of these new computational operators is expected to provide new design tools for more durable coatings for turbine blades and for longer-lived performance, especially in sandy environments.
WAY AHEAD

The contact angle at the coating–turbine blade interface is important because it tells us about the wettability of the material coating, which is related to blade wear, especially in sandy environments (Figure 2). So capabilities for prediction, engineering design, and control of the contact angle in coatings are of great importance. DEVCOM ARL scientists, Dr. Ghoshal and Dr. Luis Bravo, plan to use these methods to formulate predictive tools for exploring the design and wear of heterogeneous functionalized surfaces. This information will then be used to guide the manufacturing of next-generation turbine blade coatings. It is known that a material that exhibits hydrophobicity (a measure of the tendency to orient toward a nonaqueous environment rather than an aqueous environment, a type of “water-repelling”) with respect to sand in the laboratory will likely perform better under engine-relevant conditions. This will be pursued as a design tool for more durable turbine blades and longer-lived performance.

SUCCESS STORY

A Mathematical Picture Language for Topological Quantum Computation

This initiative in TQC, a fault-tolerant robust computational paradigm for hard-to-solve computational problems, has resulted in a novel pictorial language that is well suited to specifying, expressing, and mathematically validating algorithms.

CHALLENGE

Quantum computation promises to provide solutions that are several orders more efficient than classical information processing. However, such computational models exploiting novel quantum physics principles are error-prone due to interference of the environment with the quantum system. Traditional circuit-based quantum computing models require a large number of additional resources to apply error corrections in order to generate meaningful computational solutions. The inherent probabilistic nature of quantum computation (Figure 3) adds an extra dimension of difficulty for computer programmers who seek to increase the probability of an accurate calculation while also developing correct, bug-free code.

Another challenge in quantum-based computation is the fact that the logic of computation is often subtle and counterintuitive. It is not easy to verify that the code is constructed according to the specification of the program. A unified framework to describe specification, instruction for execution, and reason with the code constructed for correctness is challenging to develop.

A third significant challenge is the extremely low-temperature regime required to operate the quantum computers, making them unsuitable for field operations.

ACTION

During a site visit to Harvard University, Dr. Myers and Dr. Radhakrishnan Balu, former acting ARO Program Manager of the Modeling of Complex Systems Program, met with several of the faculty and chatted about what ideas they had under consideration in this area of computational sciences. The idea for a pictorial approach to computation and, in particular, to the combinatorially complex problems arising in quantum information processing, was discussed. Also discussed were the possibilities of supporting work in this area with Dr. Sara Gamble as the ARO Program Manager for Quantum Information Science. Drs. Myers, Balu, and Gamble developed a MURI topic in the area,

Figure 3: In the simulation S1, a 90° rotation of pictures represents Fourier transformation and takes multiplication to convolution, giving a geometric, picture proof of reflection positivity.
ARL Competencies:

- Network, Cyber, and Computational Sciences
- Photonics, Electronics, and Quantum Sciences

CHAPTER 3  
SUCCESS STORIES

ARL Competencies:

Results

- Developed a pictorial topological quantum programming language, 3D Quon.
- Enabled collaboration between Professor Jaffe’s theory group and ARO-funded experimental physicist Professor Misha Lukin (Harvard University) to realize the building blocks of the new language.

Anticipated Impact

3D Quon is expected to help enable future leap-ahead technologies such as securing communication of critical information, processing data from hypersensitive quantum sensors, and helping discover novel designer materials relevant to protective gear for Soldiers.

Figure 4: 3D Quon quantum teleportation protocol, generalizing the most commonly used quantum communication protocol of Bennett.
This work combined topological data analysis (TDA) and dynamical data embedding to cluster and extract distinct locomotion behavior from video data of a commonly studied worm, C. elegans.

**CHALLENGE**

While recent advances in machine learning (ML) have enhanced Soldiers’ abilities to process large and complex data, this progress remains reliant on both the abundance of data and the computational power necessary to train the associated models. This training is a time- and resource-intensive process poorly suited for the novel, unlabeled, and limited data often encountered in time-critical applications, such as in the automated extraction and classification of behaviors from video. Much of this training effort results from learning to overcome trivial differences in the data irrelevant to the task. The goal of TDA is to apply tools from algebra and topology to robustly distill complex, high-dimensional behaviors.

**SUCCESS STORY**

Robust Classification of Locomotion Behaviors Using Topological Data Analysis

This work combined topological data analysis (TDA) and dynamical data embedding to cluster and extract distinct locomotion behavior from video data of a commonly studied worm, C. elegans.

**CHALLENGE**

While recent advances in machine learning (ML) have enhanced Soldiers’ abilities to process large and complex data, this progress remains reliant on both the abundance of data and the computational power necessary to train the associated models. This training is a time- and resource-intensive process poorly suited for the novel, unlabeled, and limited data often encountered in time-critical applications, such as in the automated extraction and classification of behaviors from video. Much of this training effort results from learning to overcome trivial differences in the data irrelevant to the task. The goal of TDA is to apply tools from algebra and topology to robustly distill complex, high-dimensional behaviors.
structures in data down to multiscale summaries that preserve the essential features of the geometry while ignoring the irrelevant dissimilarities caused by noise and trivial transformations. However, current methods in TDA provide a summary of “the shape of the data” that is difficult to interpret. The goal of this effort is to recover human-interpretable versions that are robust and intuitive.

**ACTION**

Continuing investments by ARO Modeling of Complex Systems Program Managers in TDA have resulted in advances by Professor Peter Bubenik (University of Florida) and others within the program toward maturing the necessary mathematical frameworks required to apply TDA techniques directly relevant to Army interests, such as the extraction of coherent biological behaviors from video.

**RESULT**

Professor Bubenik’s team, in collaboration with researchers from the Georgia Institute of Technology’s School of Chemical and Biomolecular Engineering, used novel TDA techniques to extract distinct locomotion behaviors from videos of a simple biological organism, *C. elegans*, from videos of that organism interacting with a variety of environmental media. Results are described in Thomas et al. (2021). Complex topologically coherent behaviors were identified, enabling tracking and rapid classification of different behaviors and transitions from videos where only few and quasiperiodic or incomplete behaviors were captured. This was accomplished by preprocessing a library of *C. elegans* locomotion behaviors by extracting the shape of the centerline profile from video data. High-relevance features of this centerline pose data were then extracted from the library of poses using principal component analysis. It was shown that only a few principal components were required to capture most of the motion behavior. The motion of the worm was then projected into trajectories in the first few principal component directions. This pipeline from video frame to low-dimensional trajectory is depicted in Figure 1 for a specific case study video.

Once the trajectory data has been extracted, a persistence diagram is constructed using filtration via Vietoris–Rips complexes. Using a sliding window embedding, four distinct persistent behaviors can be extracted from the case study video, as shown in Figure 2. These four behaviors, backward, forward, pause, and transition, were identified by their prominence in the persistence diagram as measured by the distance perpendicular to the diagonal birth=death line, where short-lived topological figures accumulate. From the behavior summary points, the associated points in the principal component trajectories can be identified, as denoted by the highlighted red segments overlaying the trajectory of Figure 2. Given these persistent features in trajectory space, the corresponding average representative motion cycles can be extracted as depicted by the green surfaces of Figure 2. An example animation of the forward behavior is also available online in the supplemental material of Thomas et al. (2021).

**Figure 1:** Example video frame from *C. elegans* microscopy (black and white) with sample spline pose created from the 100-element angular partition of centerline (green curve) and 2D projection of *C. elegans* motion trajectories into the first three principal component mode amplitudes (PC1, PC2, PC3) extracted from a video library of pose shapes.

**Figure 2:** Comparison of top-four most persistent *C. elegans* behaviors: backward, forward, pause, and transition. Highlighted points on persistence diagram are associated with labels and highlighted trajectory regions correspond to topologically persistent features of motion. Green surfaces represent characteristic quasiperiodic 2D motions of worms with time axis perpendicular to the tan surfaces.

**ARL Competencies:**

Results

- Created a novel data pipeline for the analysis and categorization of complex topologically persistent spatiotemporal behaviors capable of identifying incomplete actions while filtering out irrelevant data features.

Anticipated Impact

High-throughput automation of robust distillation of data for complex nonlinear dynamical behavior into succinct and interpretable summaries is critical to the viability of higher-level analysis for large complex physical, biological, and sociological systems.
WAY AHEAD

The method will be applied to other more-complex biologic locomotion to explore the capacity for extraction and tracking of coherent behaviors in video, particularly in the presence of additional confounding influences. This will require further automation of the preprocessing phase of the data pipeline. The technique may also be extended and applied to dynamic behaviors in other domains like flame liftoff for extracting and summarizing quasiperiodic and multiscale dynamic behaviors that emerge and defy traditional data analysis approaches. The ability to nonlinearly compress and extract relevant features of large and dynamic data streams is expected to play a critical role in the construction of future data-driven dynamical reduced-order models of complex phenomena central to the current program objectives.

SUCCESS STORY

Integration of Topological Functional Units into Deep Learning Architecture

A TDA-based functional unit was built and incorporated in the TensorFlow ML package (Google, 2015) to enable rapid integration of topological summaries of structures in ML tasks.

CHALLENGE

Artificial intelligence (AI) may facilitate teams of Soldiers and agents to cooperate so that tactical decisions will be made accurately and quickly. AI-enabled agents typically rely on estimating Soldiers’ states as measured by complex data (e.g., physiological signals). While general neural network architectures of sufficient size and complexity can be trained to recognize arbitrarily complex data structures, the amount of data required and the computational cost of the training may be quite high with no theoretic upper bound. This challenge is exacerbated by the multimodal, multisensory, multiscale, nonlinear, nonstationary, and noisy (M3N3) nature of physiological signals. It has been conjectured that a significant fraction of this cost in data and computation results from training the network to ignore noise and trivial differences such as rigid-body translations and rotations. While network structures such as convolutional neural networks are commonly used to mitigate this challenge, identifying additional theoretically well-motivated approaches derived from the natural geometric structures of data has the potential to significantly mitigate these costs while providing more robust and interpretable results.

ACTION

ARO investments by Modeling of Complex Systems Program Managers Drs. Myers, Balu, and Martin have helped mature the field of statistical TDA to enable integration with existing ML technologies. By relying on theoretically persistent topological summaries of data in learning pipelines, ARO hopes to enable discovery of new classes of efficient ML techniques with rigorous mathematical foundation.

RESULT

Professor Vasileios Maroulas’ team (University of Tennessee, Knoxville) developed a topological functional unit (ToFU) (Oballe et al., 2021) with response dependent on the similarity of data topology measured by matching and computing distances between points in the space of persistence diagrams. Persistence diagrams, a multiset collection of points, are topological summaries of the shape of data. However, such points are naturally unordered, and the significant features, which reveal the central characteristics of the shape of data, must first be matched before the degree of dissimilarity can be meaningfully measured. To do this, the team developed a minimal-cost matching function:

\[
\min_{\gamma} \sum_{p \in \mathcal{D}} \| p - \gamma(p) \|_2^2
\]

Equation 1, reminiscent of the Wasserstein distance from optimal transport, is applied in the space of persistence diagrams. A representation of the distance is given in Figure 3. Once the permutation of points that minimize the mismatch is determined, the comparison of persistence diagram distance in birth–death space of topological features is stabilized independent of the arbitrary index ordering. Because the minimal matching index function is stable almost everywhere, the gradient of the cost, \( d\mu/d\mathcal{D} \), can be computed for parameterized
persistence diagram representations enabling integration with existing stochastic gradient descent-based ML methods.

With this formulation, a ToFU module for computing this minimal-cost matching was integrated in the TensorFlow deep learning framework for incorporation into general learning tasks. Figure 4 depicts the impact of adding the ToFU unit into a variational autoencoder (VAE) architecture clearly showing the improved interpretability of the topologically aware artificial neural network in an image classification task. This improved interpretability also corresponded to quantitatively enhanced classification power. Performance was demonstrated to rival that of manually tuned topological features while exceeding those of traditional black-box neural network architectures. This performance demonstrates the potential impact of automating the exploitation of fundamentally robust topological features already present in data from complex systems.

WAY AHEAD

Professor Maroulas is collaborating closely with DEVCOM ARL researchers at the Human Research and Engineering Directorate at Aberdeen Proving Ground (APG) as a Senior Research Fellow. There, he is applying and extending these techniques to synthetic physiological data provided by the APG team. Professor Maroulas also plans to develop a Bayesian analog of the aforementioned tools so that experimental data are used to update the theoretical findings. If successful, these techniques will enable processing large-scale neuroscience data on electroencephalography and electromyography as ways of untangling brainwave activities for physiological state estimation to enhance human–machine interactions. He has also been invited to speak at an upcoming United States Military Academy (USMA) Colloquium on Computational Engineering Mathematics and Data Science in hopes of engaging cadets in the future development and experimentation to develop these data analysis approaches. Through these interactions, Professor Maroulas seeks to seed an ecosystem of cadets and civilian undergraduate and graduate students who will work hand-in-hand with DEVCOM ARL scientists along with faculty from USMA and other universities on Army-relevant research focused on the emergent national challenges in the development of AI, thereby securing the U.S. prominence in this area.
COMMUNICATIONS AND HYBRID NETWORKS PROGRAM

Program Manager
Dr. Robert Ulman

Dr. Ulman received his B.S. from the Virginia Polytechnic Institute and State University in 1984, M.S. from Ohio State University in 1986, and Ph.D. from the University of Maryland in 1998, all in Electrical Engineering.

He came to ARO in 2000 as the Program Manager for Wireless Communications and Networks. He spent three years (2017-2020) as a Program Manager in the ARO International Office London.

CURRENT SCIENTIFIC OBJECTIVES

1. Determine the fundamental limits on the capacity and secrecy in shared wireless networks that, if successful, could enable future technologies that will maximize the use of the available spectrum in congested and contested environments while ensuring secure communications.

2. Develop methods for timely gathering, delivering, and processing of critical battlefield information that, if successful, could enable information superiority and situational awareness for command control.

3. Achieve reliable quantum networking capabilities that, if successful, could enable secure and accurate sensing and communication capabilities.

SUCCESS STORY
Ultra-Low Latency Research for Wireless Multi-Hop Networks

Low-latency communications are important in tactical communications for timely decision-making and real-time control. This research has led to new algorithms to improve low-latency communications in tactical networks for data that improve latency, accuracy, and the number of data packets delivered, which could lead to faster and more accurate situational awareness on the battlefield.

CHALLENGE

Timely data from sensors are critical for battlefield situational awareness and real-time control. Current algorithms are typically designed for wired networks, with possibly a centralized single-hop connection, typical of a cellular or Wi-Fi network. However, multi-hop connections over unreliable wireless links with interfering data flows, which are typical of tactical communications network, create a very difficult problem for receiving timely data.

ACTION

Dr. Derya Cansever (now ARO acting Multi-Agent Network Control Program Manager) realized the need for new low-latency communications within a wireless multi-hop environment for real-time video to enable better situational awareness and low-delay sensor data for fog/edge computing. From previous ARO-sponsored research, Dr. Cansever recognized that Professors I.-Hong Hou and P. R. Kumar (Texas A&M University) had the analytical background to make a strong contribution in this area for the Army. Therefore, he suggested they develop a proposal, based on their grant’s research, but directed more toward the application of real-time communications in multi-hop networks. The objective of the resulting proposal is to establish a new framework for developing network algorithms that ensure both end-to-end delay and end-to-end quality of experience for delivery of real-time video and other time-critical information in battlefield networks in the presence of event-driven Internet of Battlefield Things applications. The proposal was funded in 2019 with Single Investigator funds.

This success was made possible by:

Drs. Derya Cansever and Robert Ulman, Network Sciences Branch

Citations:

RESULT

This grant has investigated several important questions in wireless low-latency communications networks, two of which are described in this Success Story. The first deals with confidence of information—that is, how confident the user is that the most recent information is accurate. The second deals with information packets that must be received within a strict deadline or the information is no longer useful.

First, confidence of information in remote sensing systems was studied. Multiple wireless sensors generate noisy information updates of various surveillance fields and deliver these updates to a control center over a wireless network. The control center needs a sufficient number of recently generated information updates to accurately estimate the current system status, which is critical for the control center to make appropriate control decisions. The goal is to design optimal policies for scheduling the transmission of information updates.

This research considers a confidence of information model that incorporates both age of information and the confidence of the data. The age of information is the time since the most recent data at the consumer was measured at the remote sensor and includes latency in the transmit queue, transmission time, and the time it takes to be replaced by more recent data. Minimizing loss of confidence, defined as not having enough data points in an interval to ensure an accurate measurement, requires the control of the temporal variance of timely deliveries for each flow. This feature makes this problem significantly different from other optimization problems that only involve the average of control variables. A simple, near-optimal online scheduling algorithm, using Brownian approximation theory, was derived. Simulation results show the algorithm significantly reduces the average age of information at the user as compared to other state-of-the-art policies.

Second, packets with strict deadlines were investigated in multi-hop wireless networks serving multiple flows (Figure 1). The analysis made use of a link-interference graph, inferred from the wireless network topology. The timely throughput of a flow is defined as the throughput of packets of that flow that reach their destination node within a specified deadline, and the weighted timely throughput of the network is the weighted average over the flows with a given set of positive weights. A new combined routing–scheduling policy was developed that was shown to be nearly optimal for the weighted timely throughput metric. This policy has the useful property that the routing–scheduling decision for an individual packet is solely a function of its location and time-to-deadline, so a wireless node does not require knowledge of the global network state. It is easily implementable in a decentralized fashion by the nodes given the attempt probabilities.

WAY AHEAD

Professors Hou and Kumar will continue to investigate low-latency algorithms, potentially incorporating recent advances they have made in multi-armed bandit reinforcement learning. DEVCOM ARL researchers have been closely following this effort, and potential collaborations will be investigated.

Results

- Developed a new networking algorithm for information with hard deadlines, leading to more packets being received before the deadline.
- Developed a new networking algorithm that combines timely information with accuracy to improve the confidence of information.
- Resulted in a Best Paper Award at the 2020 ACM MobiHoc conference.

Anticipated Impact

New low-latency protocols for battlefield communications will lead to more timely data for improved decision-making.
SUCCESS STORY

Networking with Massive Multiple-Input Multiple-Output (MIMO)-Enabled Millimeter-Wave Communications

New machine learning (ML)-based millimeter-wave communications algorithms significantly enhance throughput by optimizing the use of large antenna arrays and scheduling.

CHALLENGE

Millimeter-wave communications is an emerging area, opening up a new spectrum. However, it requires highly directional antennas and is much more prone to blockage than more conventional communications at lower frequencies. Massive element arrays that are possible with the higher frequencies of millimeter-wave communications create new opportunities for fine-grained directional control of the RF beam and give the added gain required for the larger path loss at those frequencies. To take advantage of this flexibility, new antenna array control algorithms that can operate in the difficult propagation environment of a mobile Army network are necessary.

ACTION

Dr. Cansever recognized the opportunities in the emerging millimeter-wave communications and the need to research the control of massive element arrays for the use in mobile Army networks. He discussed this problem with Professor Robert Heath at the University of Texas at Austin, who had been working on an ARO Single Investigator grant investigating millimeter-wave propagation in a cluttered environment. Dr. Cansever realized that there is great opportunity to optimize the use of massive element array antennas at millimeter-wave frequencies. These massive element arrays are made possible by the short millimeter waves and help overcome the higher path loss in this frequency band. He suggested Professor Heath leverage his past research on millimeter-wave antennas and propagation, and investigate new ML algorithms for joint array adaptation and scheduling to account for, and even take advantage of, the changing propagation environment and blockages caused by motion.

RESULT

This research created a new moving millimeter-wave massive MIMO framework with configuration steps for scheduling and link configuration (Figure 2). The framework includes a novel beamforming algorithm to optimize beam codebook and beam selection to improve performance. First, overall user scheduling is optimized to maximize the use of the spectrum. Next, relay selection is performed for destinations that are blocked by obstructions. Finally, tracking is performed, if necessary, for mobile nodes.

Optimal beam selection for massive MIMO to maximize performance can be a difficult problem due to the large number of possible configurations. To make beam selection more tractable, the problem can be divided into codebook selection—considering and selecting which beams should actually be used. A codebook with many narrow beams delivers a higher antenna gain leading to higher throughput, but fewer wider beams require less scanning time to investigate and fewer reconfigurations in the cases of rapid motion or environmental changes. A novel ML approach was investigated using two stages: codebook beamwidth selection followed by actual selection of one or more beams within the codebook. The resulting algorithm uses a novel two-layer multi-arm bandit reinforcement learning algorithm, with the upper bandit selecting the codebook and the lower bandit selecting the beams. The optimization of the codebook balances the additional gain from many narrow beams and the overhead to select and track using the receiver. The resulting Thompson sampling–based algorithms improve convergence time over previous algorithms as well as significantly reduce the throughput performance gap to bounds based on perfectly knowing the channel state.

Millimeter-wave networking was further investigated by considering jointly and dynamically scheduling users, and configuring links to minimize the system delay. This research investigated how user scheduling and millimeter-wave link configuration are mutually affecting each other and if there is a solution that can jointly solve both of them. To solve this complex scheduling problem, it is modeled as a dynamic decision-making process, and two reinforcement learning–based algorithms were developed to control the resulting process. The first solution is based on deep reinforcement learning (DRL), which leverages the proximal policy optimization to train a neural network–based solution. Due to the potential high sample complexity of DRL, a multi-armed...
bandit–based approach was also researched, which decomposes the decision-making process into a sequence of subactions and exploits classic maximum weight scheduling and Thompson sampling to decide those subactions. Simulation results showed significantly reduced queue lengths that result in reduced delays for the end user.

WAY AHEAD

The team plans to continue research on millimeter-wave antenna optimization and scheduling, particularly investigating relays, moving toward multi-hop networking. Transitioning opportunities of this millimeter-wave technology to the DEVCOM C5ISR Center will be investigated.

Figure 2: Notional massive MIMO millimeter-wave wireless mobile communications network.

Results

• Developed new antenna optimization algorithms that take advantage of the flexibility of millimeter-wave antennas and new schedule algorithms.
• Resulted in a Best Paper Award Runner-up at the 2021 ACM MobiHoc.

Anticipated Impact

The exploitation of emerging millimeter-wave communications technology is expected in future battlefield networks to take advantage of the large bandwidth. This research into novel medium access control and networking algorithms will lead to improved operational performance in these future systems.
Building the Scientific Foundations for Adaptive Cyber Defense

Investigations and investments in the scientific foundations of dynamic cyber systems led to the creation of analysis tools and metrics that can perform resiliency, agility, and performance tradeoffs, and help guide both proactive adaptation and reactive response against present and future attacks.

CHALLENGE

Today’s cyber defenses are largely static and governed by slow deliberative processes involving testing, security patch deployment, and human-in-the-loop monitoring. As a result, adversaries can systematically probe target networks, pre-plan their attacks, and ultimately persist for long times inside compromised networks and hosts. In response to this situation, researchers started to investigate various methods that make networked information systems less predictable, with concepts such as using Moving Target Defenses (MTD) to dynamically change our systems (Figure 1) or adopting artificial diversity in system composition and configurations. Unfortunately, the majority of this research has been focused on developing specific new techniques as opposed to understanding their overall operational costs, when they are most useful, and what their possible interrelationships might be. Moreover, these approaches assume stationary and stochastic, but non-adversarial, environments. Situations with intelligent peer adversaries operating in a fast-changing networked environment produce dynamic behaviors that violate their assumptions.
ACTION

After identifying the critical need in establishing the scientific foundation and framework for proactive cyber defense through systems adaptations instead of ad hoc actions, Dr. Wang took quick actions to jumpstart research. Dr. Wang organized two ARO special workshops to bring key researchers together to share their research ideas, identify research challenges, and define roadmaps. He launched a Multidisciplinary University Research Initiative (MURI) project that combines multidisciplinary research efforts from network, computational, and cognitive sciences, in conjunction with optimization and operations research. He also initiated and maintained a close collaboration between the MURI team led by Professor Sushil Jajodia (George Mason University) and the DEVCOM ARL C5ISR intramural research and DEVCOM C5ISR cyber-defense teams. The MURI team not only generated highly cited research papers, but also created patented technologies, such as a disposable virtual work system and a novel malware detector, which were transitioned to DEVCOM C5ISR. In addition, the MURI team has worked with the DEVCOM ARL cyber-defense operational team to jointly develop optimized resource allocation schemes that greatly enhanced the effectiveness in alert monitoring and cyber-incident management.

RESULT

Under the ARO Cyber Adaptation MURI project, Professor Jajodia and his colleagues started to investigate adaptation techniques (ATs) that make networked information systems less homogeneous and less predictable. The basic idea was to engineer systems that have homogeneous functionalities but randomized manifestations. Homogeneous functionality allows authorized use of networks and services in predictable, standardized ways, while randomized manifestations make it difficult for attackers to engineer exploits remotely. This research has yielded a rich repertoire of AT methods for introducing diversity and uncertainty into networks, applications, and hosts. Moreover, they investigated the criteria for deciding where, when, and how to best employ available AT options. Such management decisions are complex due to the performance and security tradeoffs inherent in AT approaches. The MURI project has harnessed a broad array of adversarial reasoning (AR) techniques to identify effective and stable strategies for deploying AT options in operational systems. AR combines ML, behavioral science, operations research, control theory, and game theory to address the goal of computing effective strategies in dynamic, adversarial environments. These techniques force adversaries to continually reassess, reengineer, and relaunch their cyber attacks. By integrating game-theoretic and control-theoretic analyses for tradeoff analysis, adaptive cyber defense (ACD) presents adversaries with optimized and dynamically changing attack surfaces and system configurations, thereby significantly increasing the attacker’s workloads and decreasing their probabilities of success.

WAY AHEAD

Building on this work, Professor Jajodia and his colleagues are exploring fundamental scientific problems essential for autonomous cyber defense, a key research thrust both DEVCOM ARL and the DEVCOM ARL C5ISR intramural research and DEVCOM C5ISR cyber-defense teams. The MURI team not only generated highly cited research papers, but also created patented technologies, such as a disposable virtual work system and a novel malware detector, which were transitioned to DEVCOM C5ISR. In addition, the MURI team has worked with the DEVCOM ARL cyber-defense operational team to jointly develop optimized resource allocation schemes that greatly enhanced the effectiveness in alert monitoring and cyber-incident management.

Anticipated Impact

The new cyber-ATs that were developed could be adopted by a cyber defender to better counter malware attacks. MTD adaptation quantification frameworks allow the cyber defenders to optimally select and combine the most cost-effective MTD techniques under dynamic, changing cyber situations. Resource optimization schemes and algorithms for cyber-defense analysts teams have been adopted by DEVCOM Cyber Security Operations Center for analyst scheduling and shift arrangement.

"To the best of our knowledge, this is the first work to fit the attack surface concept to the network level as a formally defined security metric. Results show that the proposed algorithms can produce relatively accurate results with a significant reduction in the costly calculation of attack surface, paving the way for practical applications at the network level.”

Professor Sushil Jajodia, George Mason University.
and DEVCOM CSISR are currently pursuing. He and his colleagues will continue to explore new research topics such as adopting game and control theory-based MTD and ACD techniques for fully autonomous cyber operations; adopting online learning algorithms, including deep recurrent networks and reinforcement learning, for the kinds of situational awareness and decisions that autonomous cyber systems will require; and using ML and cyber-deception methods to reason about the situation and appropriate responses.

SUCCESS STORY


The ARO MURI research on cyber deception has successfully created computationally enabled models that can capture individual cognitive characteristics (biases and saliency) in decision-making, which is critical for the integration of the human component with AI/ML techniques for maximizing effectiveness of cyber defense.

CHALLENGE

The decision-making process of cyber defenders protecting computational systems and information networks is highly specialized and complex. Cybersecurity tools involving AI/ML techniques help support traffic monitoring, filter out data, and organize large amounts of network events by preprocessing and classifying data in an effort to reduce the information workload of human analysts. However, multiple limitations in the current technologies for cyber defense remain, including that most current defense strategies are static, they generate a large number of false positives, they do not adapt according to the status of the network, they do not consider predictions of potential actions of attackers and regular users of the network, and ultimately they do not support the work of human analysts appropriately. On the other side, cognitive models are generative, in the sense that they actually make decisions in similar ways like humans do based on their own experience, rather than being data-driven and requiring large training sets. In this regard, cognitive models may be better suited for assisting cyber-defense decision-making. The key challenge is to create quantitative and robust models of human cognitive decision-making that can be used in conjunction with AI/ML-based approaches that can incorporate experiences and lessons learned from past interactions, and extract cognitive saliency from individual players for making better on-the-target decisions and individualized deception projections.

ACTION

Dr. Wang has been an advocate and champion of cyber-deception research for the past several years. He has organized several workshops on cyber deception to identify the research challenges and help define critical research thrusts. Realizing that successful cyber deception relies on a good understanding of our adversaries, he emphasized the importance of incorporating cognitive research in many of his talks (including keynote speeches at several national and international conferences). He formulated the multidisciplinary topic of cyber deception and successfully launched the project in 2017. Under the ARO Cyber Deception MURI, Professors Cleotilde Gonzalez and Christian Lebiere of Carnegie Mellon University (CMU) are leading the cognitive sciences research thrust. Dr. Wang has facilitated the collaboration of the MURI team with Dr. Allison Newcomb, who leads the DEVCOM ARL CyberVan test and evaluation facility.

"The present study is the first to calculate cognitive salience to introspect into the model how humans weigh the contextual features in their decisions, and how the representation of features can influence decisions.

An instance-based learning cognitive model, built in ACT-R, accurately predicts human performance and biases. The present research shows that we can leverage the predictive power of a generalizable IBL model to infer an individual’s knowledge, trace their experience, and exploit their biases to design an adaptive signaling scheme that is personalized."

From Cranford et al. (2020)
RESULT

As mentioned, cognitive models are generative, making decisions based on their own experience, rather than being data-driven and requiring large training sets. In this regard, cognitive models differ from purely statistical approaches, such as ML, that are often capable of evaluating stable, long-term sequential dependencies from existing data but fail to account for the dynamics of human cognition and human adaptation to novel situations. Under the Cyber Deception MURI project, Professors Gonzalez and Lebiere have generated theoretically grounded cognitive models that “clone” human memory (of end users, attackers, and defenders) by tracing human actions and predicting the next human decision. These models are dynamic and adaptable computational representations of the cognitive structures and mechanisms involved in tasks such as cyber decision-making under conditions of partial knowledge and uncertainty. They have demonstrated this approach in a wide variety of testbeds, ranging from very simple and abstract to highly complex and realistic in the context of cybersecurity.

In a recent study, the CMU researchers have shown the effectiveness of such approach by creating a cognitive deception signaling strategy, which in contrast to traditional approaches, is adaptable to human actions and can be personalizable to individual attackers to provide new dynamic capabilities for cyber defense (Figure 2). Although a game-theoretic model may help provide deception signaling schemes based on the model assumption, in the real world, adversaries’ attack choices and actions are always found to vary widely. Examining salience with cognitive models helps gain valuable information about individual differences among attackers. Results from this study provided unique insights on how an individual weighs important factors such as reward and penalty in their decisions, how information is processed, and how it impacts decisions, which are critically important for helping defenders to deploy adaptive and target-specific deception for maximum effectiveness.

WAY AHEAD

Professors Gonzalez and Lebiere will continue to investigate how computationally enabled cognitive clones can influence ML/AI algorithms directly and how they can help create personalized deception strategy for highly effective cyber defense. They also expect to explore and advance the science of human–AI teaming by creating a cognitive model that will help optimized collaboration among AI, cognitive clones, and humans by leveraging the complementary strengths of humans, AI, and cognitive models.
SUCCESS STORY
Graphical Games and Distributed Reinforcement Learning Control in Human-Networked Multi-Group Societies

This ARO initiative has indicated that anomalous behaviors of interacting autonomous systems can be detected and corrected using a data-driven method of inverse reinforcement learning (RL), even when detailed technical knowledge of the autonomous system models is not known in advance.

CHALLENGE
Autonomous systems, such as autonomous driving vehicles, mobile robots in logistics, and remote medical robots, must perform according to their normal desired behaviors. However, autonomous systems are often complex and may act differently from their expected behaviors due to malicious attacks or software and hardware problems. Thus, it is significant for the autonomous systems to detect their anomalies and recover to normal behavior without necessarily requiring human intervention. Currently used anomaly detection methods are not universal, there are no methods that can detect and correct all possible types of anomalies, and they are generally not suitable for real-time operations.

“We develop inverse reinforcement learning (RL) to provide a rigorous framework for anomaly detection in differential dynamic autonomous systems for the first time. Inverse RL is applied to both the normal nominal system and an observed test system to learn and compare their objectives and control intentions in the training phase and detection phase, respectively.”

Professor Frank Lewis, University of Texas at Arlington
**ACTION**

Dr. Cansever identified RL as an important research area for the Army. He met with Professor Frank Lewis, an expert in decision learning at the University of Texas at Arlington, during the IEEE Decision and Control conference. They had a discussion on open research problems in RL and decided to organize an ARO-sponsored workshop. Based on the discussions during the workshop, Dr. Cansever encouraged him to submit a white paper to ARO on behavior detection in RL. The white paper and ensuing proposal led to an ongoing ARO project, “Graphical Games and Distributed Reinforcement Learning Control in Human-Networked Multi-Group Societies.”

**RESULT**

To overcome the challenge of anomaly detection in autonomous systems, Professor Lewis proposed a unified framework for several types of anomalies and false alarms in autonomous robotic systems described by differential dynamics (Figure 1). Professor Lewis and his team considered a normal system with nominal behaviors and an observed test system that may exhibit anomalous or abnormal behaviors. They used inverse RL to reconstruct the nominal objective function and control intention of the normal system. Then, they further used inverse RL to determine the objective function and control intention of the observed test system. The obtained objective and intention of the observed test system are compared with that of the normal system. Thus, various types of abnormal and abnormalities are identified. Correction is further executed after abnormalities are found. They provided a unified framework for several types of anomalies and false alarms in autonomous systems including noise anomaly, objective anomaly, intention anomaly, abnormal behaviors, noise-anomaly false alarms, and objective false alarms. They developed an inverse RL algorithm to reconstruct the objective and control intention of a system to be used in the training phase. Both model-based and model-free inverse RL algorithms were designed. The algorithms have two parts, optimal control learning by RL and inverse optimal control learning. Inverse RL is applied to both the normal nominal system and an observed test system to learn and compare their objectives and control intentions in the training and detection phases, respectively. Then, anomaly correction is executed for the correction phase based on the proposed inverse RL algorithms (Figure 2). They provided a rigorous analysis of the problem, proved convergence of the proposed algorithms, and demonstrated their effectiveness using simulations.

**WAY AHEAD**

This work is pursued in close collaboration with scientists from DEVCOM GVSC, resulting in a joint paper describing part of the results of their collaboration. Part of the research results are being tested by the Ford Motor Company for potential transition to Ford’s autonomous vehicles. If successful, this research is expected to be transitioned to DEVCOM GVSC and DEVCOM ARL CISD.

**SUCCESS STORY**

**Adversarial Signal Processing and Inverse Cognitive Sensing**

This ARO initiative has identified methods on how to detect if a sensor is cognitive and how an object that is tracked by a cognitive sensor can mask its actions. Conversely, this work is also applicable for the operation of a smart sensor in masking its cognitive abilities.

**CHALLENGE**

This research addresses the fundamental challenges in warfare that involve advanced observation systems such as smart sensors: When is an autonomous agent subject to sensing by a smart adversarial sensor? How can it infer the goal of the sensor? What can it do to ensure that the adversary is confused and cannot take the correct sensing action? The answers to these questions are critical to hide our sensing capabilities from adversaries.

**Anticipated Impact**

The outcome of this research could potentially increase the safety and security for autonomous systems such as the Next Generation Combat Vehicle.
ARL Competencies:

This success was made possible by:

Dr. Derya Cansever,
Network Sciences Branch

Citations:


Results

- Developed inverse filtering algorithms to estimate an adversary sensor’s gain.
- Derived inverse cognitive sensing methods to identify an adversary’s utility function.
- Designed methodologies for smart interference to counter an adversary’s maneuvers.
- Derived necessary and sufficient conditions to identify optimal sequential decision-making and estimate costs of an adversary agent.

Anticipated Impact

The outcome of this research can potentially enhance the performance and effectiveness of cognitive radar systems used by the Army.

ACTION

After having identified RL as an important research area for the Army, Dr. Cansever was concerned about the mutual impact of interacting, noncooperative, and possibly hostile RL agents, and the implications of this paradigm for the Army. He met with Professor Vikram Krishnamurthy, an expert in RL and game theory at Cornell University. They had a discussion on how interacting RL agents can learn or hide their interactions from each other, and how this could impact the Army. Based on these discussions, Dr. Krishnamurthy submitted a white paper to ARO on inverse cognitive sensing. The white paper and ensuing proposal led to an ongoing ARO project, “Adversarial Signal Processing and Inverse Cognitive Sensing.”

RESULT

Using ideas in inverse Bayesian filtering, inverse RL, and stochastic optimization of dynamical systems, Professor Krishnamurthy addressed the following questions in an interactive RL environment: (1) By observing its decisions, how can one detect if the adversary agent is a utility maximizer? (2) How can one identify if its decisions are consistent with an optimal controller? (3) How can one purposefully modify actions to confuse an inverse learner? To address these goals, he adopted fundamental results from Langevin dynamics in dynamical systems, inverse RL in ML, and Bayesian revealed preference in economics. He used these tools to design a smart sensor that can mask its cognitive abilities and developed novel tools in radar design. He developed inverse filtering methods to estimate the adversary’s sensor gain, developed inverse cognitive sensing techniques to identify adversary’s utility function (goal), and designed smart interfaces to counter the adversary’s maneuvers (Figure 3). To achieve these results, he constructed interpretable Bayesian utility maximization models that behave identically to deep convolutional neural networks (Figure 4). He derived necessary and sufficient conditions to identify optimal sequential decision-making and estimate costs of the decision maker, and established equivalence between classical and Bayesian revealed preferences in microeconomics.

WAY AHEAD

This work initiated close collaborations between the principal investigator and DEVCOM ARL scientists to conduct research on radar technologies. If successful, this effort could lead to novel sensing technologies for the Army.
SOCIAL AND COGNITIVE NETWORKS PROGRAM

Program Manager
Dr. Edward T. Palazzolo

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. at the University of Illinois Urbana-Champaign in 2003 in Organizational Communication and Knowledge Management.

He came to ARO in 2014 as the Program Manager for Social and Cognitive Networks.

SUCCESS STORY
Predictive Modeling for Early Identification of Suicidal Ideation in Social Networks

Researchers discovered a way to leverage machine-learning (ML) and decision-tree techniques to better understand and predict suicidality among homeless youth. Numerous social network characteristics were found to be prominent correlates of suicidal ideation and can be used to form an early identification process for at-risk active duty Soldiers and veterans to reduce suicidal behaviors.

CHALLENGE
Although we know social networks can influence an individual’s behavior, current work suffers from the limitations of standard statistical analysis to deeply understand the ways social networks and individual psychological profiles combine to predict individual behaviors. This intersecting space is critical to understand, especially with respect to reducing suicidal ideation and suicide attempts.

It will take an interdisciplinary team of computer scientists and social scientists to discover novel modeling strategies.

ACTION
In 2015, Dr. Palazzolo met Professors Eric Rice and Milind Tambe, co-founders of the University of Southern California’s (USC’s) Center for Artificial Intelligence in Society at a program review for the Game Theory Multidisciplinary University Research Initiative (MURI) (led by Professor Tambe and managed by ARO’s Dr. Purush Iyer). Dr. Palazzolo was inspired by Professor Rice’s talk and focus on

CURRENT SCIENTIFIC OBJECTIVES
1. Discover the fundamental principles governing human teaming activities that support designing and maintaining high-performance teams that, if successful, will allow the Army and Joint Staff to engineer high-performance teams with specified characteristics to satisfy mission requirements and enable teaming with unprecedented coordination across multiple defense organizations, while improving Soldiers’ cognitive resilience.

2. 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 pinpoint accuracy, especially with potential for real-world effects, to support Army and Joint Operations by providing support for decision-making.

3. Create new social network research methods and analytics to handle the challenges associated with novel and advanced research in team science and computational social science that, if successful, will enable deeper understanding of the complex human terrain in Multi-Domain Operations.

This success was made possible by:
Dr. Edward T. Palazzolo, Network Sciences Branch

Citations:
artificial intelligence (AI) for social good and invited Professor Rice, an associate professor of Social Work, to submit a social science–focused proposal that could leverage ML techniques to address the challenge of suicidal ideation. The 2016 proposal “Predictive Modeling for Early Identification of Suicidal Thinking in Social Networks” was selected for funding in 2017.

During a midpoint review, Dr. Palazzolo was impressed by their theoretical and mathematical models to understand suicidal ideation among homeless youth, and encouraged the research team to work with an active military unit to collect pre- and post-deployment data to assess the validity of this process for identifying at-risk Soldiers, and then mitigate that risk, if possible. Professor Carl Castro, a professor of Social Work at USC, retired Army Colonel, and co-principal investigator (PI) on this research team, was able to get command approval to work with an active duty unit at an Army Post for pre- and post-deployment data collection for research on suicidal ideation. Unfortunately, after collecting pre-deployment data with 242 active duty service members, this data collection was interrupted by the COVID-19 pandemic and the unit’s deployment was extended.

Aware of the challenges the research team now faced, Dr. Palazzolo proactively solicited a one-year add-on proposal from Professor Rice to capitalize on their opportunity to collect data with the active unit. This add-on enabled the team to collect data on new stressors the team now faced with the novel coronavirus.

RESULT

This interdisciplinary team of social scientists and computer scientists pioneered a novel methodology to combine ML techniques with decision-tree analyses to test social science theories. They applied this methodology to predictive modeling of mental health (suicidal thinking, suicide attempts, post-traumatic stress, and depression) and its connection to social networks over time among active duty service members and young people experiencing homelessness.

This is the first known study to leverage ML to better understand and predict suicidality among homeless youth. Leveraging an existing dataset of 940 young people experiencing homelessness (ages 13 to 29) in Southern California, the team applied their novel Machine Learning–Decision Tree (MLDT) technique to reduce the 117 theoretically relevant, independent variables down to the seven individual (depressive symptoms, severe depression, and age first homeless) and social network (home/friend network size, network objection to risky behavior, witnessed/experienced trauma, and physical fight) variables with the most predictive power for suicide attempts. The MLDT method bifurcates the tree such that it maximizes the similarity within each node while simultaneously maximizing the differences between nodes across a spectrum of cut-points.

The MLDT analyses revealed the highest-risk profiles as a function of a nonlinear combination of factors that would not have been possible to discover using traditional methods. As shown in Figure 1 (boxes 8 and 12), the MLDT method showed that of the youths who made at least one suicide attempt, 75% reported low depression, were younger (less than 16.5 years old at first homelessness), and had experienced high levels of violence, showing that not all suicidal people are depressed.

87% reported high levels of depression, low levels of trauma, and have severe depression, showing that low trauma exposure is not sufficient to protect against suicide attempts.

In addition to the homeless youth study, the research team recruited active duty Soldiers from an Army Post in December 2019 to conduct pre- and post-deployment data regarding the Soldiers’ networks, psychological characteristics, and stressors to test their model with respect to suicidal ideation and risk. In response to the COVID-19 pandemic, the team collected data in February 2021 from 94 of the 242 post-deployment members on the psychological stressors that they were facing as a direct result of the pandemic and about their new worries regarding COVID-19 during their 2020 deployment (results summarized in Figure 2). These stressors, along with other factors, can be used in future MLDT analyses.
Next steps for this research involve the Army Resilience Directorate testing this MLDT technique on larger datasets of Army personnel to identify nonintuitive connections among individual psychological characteristics, social network information, and unique stressors on Soldiers. If successful, this work will be shared with colleagues at the Walter Reed Medical Center.

This work serves as a seedling effort to demonstrate the feasibility of computational social science research to build Community Cognitive Resilience (CCR). CCR will be a new thrust in social and cognitive networks beginning in 2022 and focuses on scientific discovery at the community level for the reduction of suicide risk, post-traumatic stress disorder, depression, anxiety, substance abuse, and susceptibility to disinformation.

**SUCCESS STORY**

**Hybrid Thinking to Support Novel Team Interactions and Collaborative Creativity**

This ARO initiative seeks to expand human creativity through the use of software agents as teammates for the development of hybrid thinking. The research team developed a new methodology for computing the novelty of an idea. Additionally, they developed a methodology for assessing the relevance of an idea by computing the probability of the idea being generated from a specific knowledge domain versus a general knowledge domain.

**CHALLENGE**

AI is often used to accomplish tasks as evidenced by arriving at a defined solution, but what if AI as part of human–agent teaming (HAT) could be used for hybrid thinking to drive humans toward more creative and novel solutions? Hybrid thinking is the process of integrating different thinking styles, and in this case, by including agents in the teaming ideation process. Early research on human teaming shows that people have a difficult time harvesting their best ideas while working in team settings. Often, team dynamics (e.g., shyness, dominance, voting, or overconfidence) lead to the most novel ideas not surviving the collaboration and decision-making process. While much has been learned about factors related to enhanced creativity, little is understood about the links between the various phases of the collaborative innovation process: collective ideation, elaboration, evaluation, selection, and development or implementation. Another challenge with the collaborative creativity process is that the team might not tap into the most creative elements of prior collaborations due to a bias for ideas that are more recent, common, or feasible rather than ones that are more radically innovative.

**ACTION**

In 2016, while on a site visit to the University of Texas at Arlington (UTA) to evaluate a grant by Professor Chunke Su, Dr. Palazzolo met with Professor Su’s colleagues from the Psychology Department, Professors Jared Kenworthy and Paul Paulus, to discuss a potential project on novelty in team-based creative ideation. Through the process of a few white-paper iterations in 2018, Dr. Palazzolo described to Professors Kenworthy and Paulus the importance of developing software agents to help human teams better perform knowledge work and that HAT was a central part of the social and cognitive networks portfolio.

Based on the feedback from ARO, Professor Kenworthy assembled an interdisciplinary team comprising himself as the lead PI and Professor Paulus, along with Professor Ali Minai at the University of Cincinnati’s Computer Science Department and Professor Simona Doboli at Hofstra University’s Computer Science Department, and submitted their proposal in 2019: “Facilitating the Survival and Development of Novel Ideas in Collaborative Innovation.” In 2020, Dr. Palazzolo selected this proposal for funding focused on the use of computer-assisted feedback to help overcome the barriers to idea survival and enhance the chances of the best creative ideas being advanced and developed.
In order to achieve the high-level goals of the grant, the research team is conducting a series of studies to develop and test a model designed to improve the relationship between collaborative creativity and the decision-making process. They are developing a unique software tool for hybrid thinking with the capabilities to (1) track the dynamics of ideation over time; (2) evaluate the ideas proposed during the creative process in terms of their topics, relevance, and novelty; (3) provide visualization of the ideation process as trajectories in the semantic space; and (4) provide real-time feedback to team members in the form of hints and suggested concepts using information about the task and strategic alerts derived from the dynamics of the thought trajectories. Ultimately, the team will test the theoretical model in conjunction with the software tool so that teams working in ideation and decision-making tasks can use the software to improve the quality of their team processes linking the ideation and decision phases. The team will test their theoretical model, which proposes key factors linking the various stages of the innovation process in conjunction with their software tool so that teams working in ideation and decision-making tasks can use the software to improve the quality of their team processes linking the ideation and decision phases.

**Results**

- Demonstrated the value of individual performer contributions to the collective ideation process.
- Discovered the optimal process for computationally modeling novelty of ideas via cognitive mapping that is robust to human raters.

**Anticipated Impact**

If successful, this research will lead to the development of a computer-assisted tool to support HATs during brainstorming processes. These HATs will aid the survival and elaboration of novel ideas in collaborative creativity and help teams avoid closed or myopic thinking.

**WAY AHEAD**

If successful, this work will demonstrate an important role for HAT in support of hybrid thinking with respect to creativity and novel thinking. While valuable in its own right, this research is even more valuable in connection with the wider social and cognitive networks portfolio’s research on transactive memory theory, collective intelligence, and artificial social intelligence. Further ensuring integration of this work with Army priorities, the research team will continue working with Drs. Cooper and Bakdash.

The early success of this research effort will be leveraged in the coming years as the team uses their work on cognitive maps to ascertain the relevance and novelty of ideas, develop a system to track and analyze the trajectory of brainstorming conversations using the cognitive map, use text salience methods from NLP to identify significant ideas in the idea stream, and collectively use this to support computer-assisted study designs during the brainstorming process. Understanding the role of individual team member contributions on quantity and novelty of ideas generated by the entire ideation team is a critical step in the development of software agents’ properties to enhance human performance.
ARMY SMALL BUSINESS TECHNOLOGY TRANSFER (STTR) PROGRAM

Program Manager
Dr. Imee Smith

Dr. Smith earned her B.S. in Biochemistry from the University of Virginia in 2003 and her Ph.D. in Bioanalytical Chemistry from the Pennsylvania State University in 2009. She came to ARO in 2021 as the Program Manager for the ARO Army STTR Program. Prior to joining ARO, she advised the Deputy Assistant Secretary of the Army for Research and Technology on emerging and priority science and technology (S&T) and technology-transition pathways as Technology Advisor and the Director of the Soldier Portfolio.

CURRENT SCIENTIFIC OBJECTIVES

1. Align the ARO Army STTR investment portfolio with Army Modernization Priorities and priority S&T research areas that, if successful, would enable new technology solutions for previously identified needs in these and other Army mission areas.

2. Continue to increase engagement with the broader technology innovation ecosystem that, if successful, would result in augmented participation in the ARO Army STTR Program from underserved communities to include more minority-owned small businesses and the Historically Black College and University/Minority-serving Institutions (HBCU/MIs).

SUCCESS STORY
Army STTR Increases Engagement with the Innovation Ecosystem through Industry Day Events

The ARO Army STTR Program hosted multiple events with innovators from small businesses, academia, industry, and nonprofit organizations in support of the Army fiscal year 2021.C (FY21.C) STTR Program Phase I cycle solicitation. These events featured opportunities for potential proposers to learn more about the ARO Army STTR Program as well as engage with ARO STTR Program Management Office (PMO) personnel, DEVCOM ARL Essential Research Program (ERP) leads, and FY21.C Phase I topic authors. Employing this strategy allowed the PMO to reach a broader audience to educate and promote the program with small businesses and research institutions across the United States.

CHALLENGE

The travel restrictions associated with the COVID-19 pandemic into 2021 proved to be challenging for traditional outreach and engagement with innovation centers across the country. Consequently, it was difficult to promote the ARO Army STTR Program and the FY21.C solicitation. These restrictions forced the ARO Army STTR PMO to develop a new, innovative way to continue its outreach mission under the constraints of a global pandemic.

ACTION

To overcome these challenges and increase engagement with potential proposers and the innovation community, the ARO Army STTR PMO devised a series of webinars culminating in an Industry Day event to promote the FY21.C Broad Agency Announcement (BAA) solicitation in collaboration with the Virginia Tech Applied Research Corporation. While an in-person Industry Day event had been held previously to promote a solicitation of a limited number of special topics in 2019, the 2021 series of engagements leveraged the now-common virtual platforms to provide not only information about ARO Army STTR and the open topics associated with the FY21.C solicitation, but also Army research priorities and the DEVCOM ARL ERPs to the general public.
This success was made possible by:

Mr. Michael Caccuitto and Ms. Nicole Fox, Technology Integration and Outreach Branch

Dr. Mohan Sanghadasa, DEVCOM AvMC

Citations:


public, targeting participation from potential proposers from small businesses and research institutions. These engagements also permitted networking between potential proposers, allowing small businesses and research institutions to engage with one another to form proposal teams. The highlight of the series was a two-day Industry Day event that featured overviews of the ARO Army STTR Program, the proposal submission and contract award process, as well as the opportunity to engage directly with topic authors from the FY21.C solicitation. Each virtual engagement was recorded and available for review following the events, allowing all potential proposers to hear the answers to questions posed by their peers even if they were not able to attend.

RESULT

The Industry Day event and the accompanying six webinars were all well attended by participants from small businesses, academia, industry, and nonprofit organizations, with 532 attendees for the two-day Industry Day event and an average of 125 participants per webinar. These events allowed the ARO Army STTR PMO to reach a much larger audience than what would have been feasible with an in-person event as there were no constraints to attendee participation. Attendee feedback was positive, with many participants finding value in the content presented and the engagement with the PMO, DEVCOM ARL ERP leads, and topic authors. In addition, networking sessions allowed researchers to engage with each other, either one-on-one or as a group, to discuss similar interests and potential collaboration.

SUCCESS STORY

Advances in Multiferroic Materials for Antenna Miniaturization and RF Applications

A team from Winchester Technologies and Northeastern University advanced the state of the art in antenna miniaturization as part of a sequential Phase II STTR-funded effort. Their work exploited the interactions between the layers of multiferroic materials in a composite structure with distinct magnetic and electric properties to produce functional miniature magnetoelectric (ME) antennas. These antennas were fabricated in the submillimeter regime, displaying higher gain versus current state-of-the-art antennas of that size.

CHALLENGE

The current state of the art in antenna miniaturization is plagued by the following challenges that limit how small an antenna can be while remaining functional:

1. Constraints for conventional small antennas imposed by Chu’s limit (the bandwidth an antenna can function in is proportional to its size) and design requirements which necessitate that an antenna’s size must be comparable to the electromagnetic wavelength, \( \lambda_0 \), often in the range of 0.1 to 0.5 \( \lambda_0 \), to operate properly within acceptable transmission loss limits.

2. Reduction in size causes antenna impedance mismatch that in turn also reduces antenna gain.

3. Susceptibility to the ground plane effects occurring when a conventional antenna (e.g., a conformal dipole antenna) is placed close to a metallic surface. This proximity generates an oppositely phased current that causes destructive interference on the electromagnetic waves radiated from the antenna, decreasing its power gain.
ACTION

A team from the DEVCOM AvMC and the U.S. Army Space and Missile Defense Command (SMDC) approached the ARO Army STTR PMO with the prospect of further advancing state-of-the-art compact antennas using multiferroic materials with additional Phase II STTR funding. This advancement would leverage previous work funded by a Defense Advanced Research Projects Agency (DARPA) STTR effort performed by a team from Winchester Technologies and Northeastern University. The ARO Army STTR Program Manager worked with DEVCOM AvMC and SMDC to develop a formal topic to be solicited against in the STTR BAA. Following the review of the Winchester/Northeastern team’s proposal for funding, the ARO Army STTR PMO selected the proposal for sequential Phase II funding in 2018.

RESULT

Building on their initial DARPA efforts, the Winchester/Northeastern team developed mechanically actuated ME antennas that are not constrained by the limitations of traditionally designed antennas and overcame the three challenges noted previously. The heterogeneous thin-film structure of these antennas permits the use of electromechanical resonance vice the electromagnetic wave resonance employed by traditionally designed antennas. This change allows these microelectromechanical systems (MEMS) antennas to be fabricated with submillimeter dimensions without the limitations encountered by the current antenna miniaturization state of the art. Fabrication in this size regime, however, brought an additional challenge to keep the structure of these antennas stable during and after assembly. To circumvent this new challenge, the team devised a method to fabricate their MEMS antennas in a solid mounted resonator (SMR)-based configuration, which not only increases the mechanical stability of these devices, but also provides robust and high-gain performance (Figure 1).

WAY AHEAD

The team continues to refine their designs and fabrication process to further miniaturize the SMR-based ME antennas, while also increasing the stability of the structures, and gain and overall system performance. These advances in the use of multiferroic materials to produce the mechanically actuated antennas pave the way for a robust multiferroics fabrication process that can be adopted by the commercial electronics community and is already compatible with complementary metal–oxide–semiconductor processing. Moreover, these miniature ME antennas can be employed for a variety of applications ranging from the biomedical industry, vehicle autonomy, and wireless communication.

Results

- Successfully designed and fabricated functional ME antennas in the micron size regime with improved gain and power handling versus current state-of-the-art. Mechanical actuation in the fabricated ME antennas yields conformal antennas with ground plane immunity and ultracompact antenna sizes comparable to their acoustic wavelength and excellent impedance matching at a small size.

Anticipated Impact

This works will lead to further miniaturization of antennas and other RF components to enable increased performance while maintaining or decreasing size, weight, and power requirements of future electronic architectures and devices.
ARO SMALL BUSINESS INNOVATIVE RESEARCH (SBIR) AND SMALL BUSINESS TECHNOLOGY TRANSFER (STTR) PROGRAM

Program Manager
Ms. Nicole Fox

Ms. Fox completed her B.A. in Business Administration at Bay Path University in 1997.

She came to ARO in 2010 as a Program Specialist contractor for the ARO Army STTR program and was hired into a government position as the ARO SBIR/STTR Program Manager in 2011. In this capacity, she manages over 100 contracts annually by supporting numerous activities through these programs to help small businesses move their technology into fully developed, tested, and commercialized products and services to benefit Army Warfighters.

SUCCESS STORY
From the Warfighter Monitor to the COVID Plus

Tiger Tech Solutions, Inc., used technology from the Warfighter Monitor (Technical Readiness Level [TRL 6]) to develop the COVID Plus Monitor. This noninvasive yet powerful tool is the first artificial intelligence/machine learning (AI/ML)-based product to receive an Emergency Use Authorization (EUA) by the Food and Drug Administration (FDA). One of the greatest advantages of the COVID Plus is that it allows users to affordably and quickly assess individuals for COVID-19 risk (Figure 1).

CHALLENGE
When the COVID pandemic first began in early 2020, very little was known about the novel coronavirus. In March 2020, Tiger Tech decided to dedicate time and effort into researching the effects of COVID-19 on the body. The team received an Institutional Review Board (IRB) approval at Mount Sinai Medical Center, Miami, Florida, for data collection on COVID-19 positive patients.

Without a proper understanding of how to treat the disease, gathering data from COVID-19 positive patients in the early days of the pandemic was extremely dangerous and required exceptional courage (Figure 2). Researchers at Tiger Tech were able to quickly identify subclinical markers unique to COVID-19 using comparative data from the Tiger Tech Warfighter Monitor database, which included tens of thousands of patients.

ACTION
Tiger Tech has developed a revolutionary monitoring device to evaluate the Warfighter’s physiological condition through the Defense Health Agency’s (DHA’s) SBIR program. The Tiger Tech Warfighter Monitor is a hands-free, continuous, real-time, multiple physiological and biomechanical wearable. The monitor is optimal for combat use as it monitors an individual’s

CURRENT SCIENTIFIC OBJECTIVES

1. Develop strong, germane, and competitive topics to stimulate technological innovation that focus on DEVCOM ARL Competences and Army Modernization Priorities that, if successful, is anticipated to lead to breakthrough research and development (R&D) that enables participating small businesses and university partners to meet federal research/ R&D needs, which they can then commercialize through sales in the private sector or back to the government.

2. Establish close ties with academia, startups, and established small businesses to achieve further insight into technology transition through funding mechanisms, program of record needs, Warfighter requirements, and Program Executive Offices (PEOs) that, if successful, is anticipated to develop methods to assist small businesses, academia, and program managers to advance the transition of their technologies to meet the needs of the Army.

This success was made possible by:
Ms. Nicole Fox, Technology Integration & Outreach Branch
Dr. Stephen Lee, ARO Senior Research Scientist
Dr. Paul Baker, Chief, Physics Branch

Citations:
biometrics and biomechanics during extreme motion, and does not require cloud computing. The IRB granted Tiger Tech approval to conduct research on COVID-19 patients. Through this continued research under an ARO Army STTR, Tiger Tech has identified three noninvasive biomarkers of COVID-19 patients. On May 2, 2020, Tiger Tech applied for a EUA with the FDA, which was granted on March 19, 2021. The Tiger Tech team continues to research the effects of COVID-19 on the body and has taken data on more than 8,000 confirmed polymerase chain reaction (PCR) positive subjects.

Ms. Fox served as co-Contracting Officer’s Representative (COR) along with Drs. Stephen Lee and Paul Baker. This effort represents a collaboration among the Army Applications Lab (AAL), ARO, DHA, and U.S. Army Special Operations Command (USASOC).

RESULT

Tiger Tech developed a noninvasive, prescreening COVID-19 wearable monitor that was derived from their Warfighter Monitor, which collected numerous direct biometric and biomechanical information, such as single-limb electrocardiogram, heart rate, heart-rate variability, pulse oximetry, pulse rate, pulse-rate variability, and temperature. They also conducted IRB-approved research at Mount Sinai Medical Center. The research was based on a normal patient baseline of +6,000 sets against +180 COVID sets. This research demonstrated hematological problems in COVID-19 patients. This resulted in the discovery of real-time, noninvasive biomarkers for COVID-19 prescreening.

WAY AHEAD

During a Phase I STTR, the Tiger Tech team used the Warfighter Monitor to identify three subclinical markers for cognitive load. This device is currently in use at the U.S. Army Aeromedical Research Laboratory (USAARL) for research on pilot performance and with Future Vertical Lift applications. The United States Marine Corps (USMC) is planning to use the Warfighter Monitor to research acute mountain sickness, dehydration, and cold-weather stress at the Mountain Warfare Training Center in a joint effort between the San Jose Innovation Unit (USMC) and the 75th Innovation Unit of AFC.

The COVID Plus has been deployed to White Sands Missile Range in support of Project Convergence 21 as a means of screening Soldiers and civilians participating in the event. The COVID Plus has been classified as a medical device by the Ministry of Health in the Kingdom of Saudi Arabia and will soon be deployed throughout that country.

SUCCESS STORY

ARO Unlocks Yellowstone Natural Products

New antivirals and antibiotics to combat COVID-19 and drug-resistant bacteria are being discovered from hot springs through two ARO/Joint Science and Technology Office for Chemical and Biological Defense (JSTO-CBD, CBD for short)/DHA SBIR projects with CFD Research
This success was made possible by:

Nicole Fox, Technology Integration & Outreach Branch

Bob Kokoska,
Life Sciences Branch

Larry Pollack, CBD Research

Citations:


Results

• Created the EMAD platform to access and screen natural products from hot springs.

• Discovered the CFD-110 novel class of antibacterial compounds.

• Developed two novel screens to find inhibitors of a COVID-19 protein.

Anticipated Impact

The natural products discovered and developed in these two SBIR projects will produce novel medical countermeasures to treat and prevent infections caused by multi-drug-resistant bacteria and coronaviruses. In addition, genetic and chemical libraries will be produced, which can be mined for future drug discovery purposes for decades to come.

CHALLENGE

Studying bacteria from hot springs has been extremely difficult due to challenges with culturing them in the lab. By isolating the DNA from hot spring bacteria and then inserting that DNA into lab-optimized bacteria, CFD Research is able to isolate novel natural products produced by this hot spring DNA. The most obvious and direct benefit for the Army using this technology will be in providing a path toward identifying new natural products with antimicrobial or antiviral properties. Beyond that, the techniques can be adapted toward identifying new temperature-stable enzymes and biomolecules that can be deployed in extreme environments and tailored for applications such as sensing, materials protection, and biomanufacturing.

More than 20 remote hot springs were sampled within Yellowstone National Park (Figure 3). These moderately thermophilic hot springs were carefully chosen to maximize biodiversity of the bacteria within the samples, which will, in turn, maximize the chemical diversity of their natural products. To further optimize the process, the Extremophilic Microbiome Antimicrobial Discovery (EMAD) platform isolated large DNA fragments (> 100 kb) to capture more complex natural product synthesizing pathways and inserted them into two hosts, which facilitate biosynthesis from thermophiles (heat-loving bacteria) (Figure 4).

ACTION

CFD Research has two active SBIR projects being overseen by Dr. Bob Kokoska (Program Manager, Life Sciences Branch) that have been making COVID waves. Based on studies that targeted the molecular mode of action, chemical modifications to the best candidate molecules were made toward improved efficacy and tested in vivo (mice models) for cytotoxicity and efficacy against biological warfare agents (BWAs). An add-on is currently near award to seek further targeted molecular modifications designed to improve stability while maintaining antimicrobial activity, paving the way for preclinical studies and an Investigational New Drug Application to the FDA. They have also successfully purified the nucleocapsid protein, and started to develop the proper incubation conditions and instrument parameters for the fluorescence binding assay (Figure 5).

Ms. Fox served as co-COR along with Dr. Kokoska. She also assisted working with other agencies to obtain additional funding to continue this necessary research. This effort also includes collaboration with the University of Oklahoma.
Currently, ARO is in the process of awarding a Phase II contract extension to this project to CFD Research to improve the stability of the most promising candidate compound by making directed changes to its chemical structure and test the efficacy of these modified compounds against BWAs in a lethal-challenge mouse model. This is expected to help meet targets for preclinical trials and an Investigational New Drug Application to the FDA. Separately, the promising results from the antimicrobial studies have resulted in a separate SBIR Pivot Sequential Phase II extension award from DHA to take the same screening protocols for used in the CBD-funded research to identify antiviral compounds, specifically compounds that can bind to and degrade the coat protein of the SARS-CoV-2 virus.

WAY AHEAD

CFD Research is attempting to develop their hot spring-derived antibiotic class, CFD-110, into an FDA-approved medical countermeasure against Francisella tularensis (which causes the high-infectious disease tularemia) and Bacillus anthracis (anthrax), both of which have a significant negative impact to force readiness, to protect the Warfighter against BWAs. Additionally, a new COVID-19 protein target is being explored to develop a novel class of antivirals from the Yellowstone National Park samples.
EDUCATION OUTREACH PROGRAM

Program Manager
Ms. Ivory Chaney

Ms. Chaney received her B.S. in 2014 and M.S. in 2017, both in Business Administration, from Liberty University. She is a certified Sexual Assault Victim Advocate for the DoD and received her certification in Project Management from Cornell University in 2020. Ms. Chaney also served 23 years in the Marine Corps Reserves with deployments to Iraq and Afghanistan.

Ms. Chaney came to ARO as the Administrative Specialist in the Physical Sciences Division. In 2021, she joined the Technology Integration and Outreach Branch as the Educational Outreach Program Specialist.

In her position, Ms. Chaney manages the Army’s High School Apprenticeship Program (HSAP) and Undergraduate Research Apprenticeship Program (URAP). She also manages Army participation in the DoD’s National Defense Science and Engineering Graduate (NDSEG) Fellowship Program; coordinates various other science, technology, engineering, and mathematics (STEM) outreach activities, including local, state, and regional events; and synchronizes efforts with DEVCOM ARL’s broader outreach program portfolio and workforce development initiatives.

CURRENT SCIENTIFIC OBJECTIVES

1. Introduce students to the Army’s interest and investment in science and engineering research through associated educational outreach efforts that support the preparation of students for the 21st-century workforce.

2. Provide hands-on research experience, through Army-funded apprenticeships, for high school and undergraduate students that, if successful, will lead to student career exploration and promote interest in STEM fields of study.

3. 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.

4. Coordinate selection of and engagement with NDSEG Fellows to maximize potential contribution to the defense research ecosystem.

SUCCESS STORY

Results-Driven High School and Undergraduate Apprenticeships

The HSAP and URAP continue to attract quality mentors and apprentices, and produce significant results for the Army in the face of the COVID-19 global pandemic.

CHALLENGE

COVID-19 continued to be a challenge for apprenticeships in 2021. Many schools were prepared to be virtual, but the release of the vaccination allowed some schools to commence apprenticeships in person or in a hybrid model. However, because of strict regulations at some universities, some labs were unable to find students to participate. Additionally, very few high school students were allowed on campus; most had virtual apprenticeships. Few undergraduates were allowed on campus on a regular basis, as well.

ACTION

To assist with these challenges, Ms. Chaney held regular meetings with the Army Educational Outreach Program (AEOP) team at the Rochester Institute of Technology (RIT) and the HSAP/URAP primary investigators to ensure they had the necessary tools to find qualified candidates. ARO extended
Anticipated Impact

The relationships built throughout the AEOp consortium, DEVCOM ARL, with the principal investigators and ARO Program Managers continue to strengthen the HSAP and URAP administered by ARO, building lasting and positive impressions of the program and the importance of science conducted for and by the DoD.

WAY AHEAD

The COVID-19 pandemic continues to help the outreach community reevaluate the way apprenticeships are advertised and conducted. Hence, the program is determined to remain flexible and agile in its ability to conduct apprenticeships under uncertain, dynamic conditions, while maintaining valuable STEM experiences for students. Ms. Chaney, along with the AEOp Consortium, have considered which programs can remain virtual or should become hybrid long into the future, thus increasing ARO’s ability to serve a diverse and inclusive community of students.
HISTORICALLY BLACK COLLEGES AND UNIVERSITIES (HBCU) AND MINORITY-SERVING INSTITUTIONS (MI) PROGRAM

Program Manager
Ms. Patricia Huff

Ms. Huff is a graduate of Howard University, receiving her B.A. in Broadcast Management in 1987. Her professional activities and accreditations include Master Certified Facilitator and Moderator (Qualitative Market 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 in communications, outreach, and stakeholder services. Early in her career, she worked in radio and television news and as a marketing research analyst for the Potomac Electric Power Company. Later, she became the owner and chief executive officer of a marketing and communications consulting company.

Ms. Huff manages and administers programs for HBCUs/MIs and other special-emphasis programs to support basic research, equipment and instrumentations investment, and other activities focused on increasing the number of underrepresented minorities in mission-critical science, technology, engineering, and mathematics (STEM) fields for the Army and the Department of Defense.

CURRENT SCIENTIFIC OBJECTIVES

1. Expand and diversify the research base and participation of HBCUs/MIs in ARO core research programs through innovative outreach and program design/execution.

2. Enhance research and engineering capabilities at HBCUs/MIs that align with Army research priorities in the fields of physical, engineering, and information sciences that, if successful, benefit long-term national security needs.

3. Provide outreach and research experiences/opportunities to faculty and students at HBCUs/MIs that, if successful, would increase awareness of Army research, partnerships, innovation, and careers leading to the next generation of world-class scientists and engineers.

4. Encourage research and education collaborations with other institutions of higher education and defense organizations.

SUCCESS STORY
Three New Centers of Excellence (CoEs) Awarded within the ARO HBCU/MI Program

DEVCOM ARL invested in three CoEs from ARO HBCU/MI Program funding. These new CoEs will conduct multidisciplinary collaborative research that will increase knowledge in the research areas of digital forensics at Florida International University (MI), environmental modeling and characterization at the University of the District of Columbia (HBCU), and extreme condition chemistry of molecular materials at the University of Illinois at Chicago (MI). These awards utilize up to 30% of the project each year as a sub-award to foster a collaborative research environment and enable connected, interdependent research efforts.

CHALLENGE

Research capacity and infrastructure at our nation’s HBCUs/MIs have lagged compared to high-tier research institutions due in part to lack of funding and associated expertise. With this challenge, it has been difficult for many HBCUs/MIs to compete for funding from both the DoD and government more broadly. Simultaneously, the pipeline of students earning a degree in STEM fields does not match the overall diversity of the nation. Without this matching diversity, it is difficult to have a diverse research base and inject innovative thought based upon different experiences. It is critical to address both of these challenges to ensure that the Army’s research and engineering needs are met by the entire academic community and also make sure its science and engineering workforce draws from and represents the nation's diversity.

This success was made possible by:

Ms. Patricia Huff and Mr. Michael Caccuito, Technology Integration and Outreach Branch
Dr. Randy Zachery, Information Sciences Branch
Dr. Cliff Wang, Network Sciences Branch
Dr. James Parker, Chemical Sciences Branch
Dr. Julia Barzyk, Mechanical Sciences Branch
ACTION

The ARO team including Dr. Randy Zachery, Ms. Huff, and Mr. Michael Caccuitto assessed past efforts to both expand and leverage investments in HBCU/MI partnerships to settle on this CoE approach. The most recent approach—the Partnered Research Initiative (PRI)—funded HBCUs/MIs through DEVCOM ARL’s Collaborative Research Alliances (CRAs) and Collaborative Technology Alliances and resulted in impactful research contributing to the overall CRA mission areas. However, it’s not clear that the PRI resulted in the long-term capacity improvement at the HBCU/MI institutions to provide the improved institutional capability necessary for conducting Army-relevant research into the future. Prior to that, the Partnership in Research Transition program funded HBCU/MI-led Cooperative Agreements with DEVCOM ARL in-house research activities in collaboration with ARO but did not generate the desired effect on HBCU/MI capacity. Going further back, the Battlefield Capability Enhancement program funded HBCU-led research centers working in collaboration with ARO and Army Battle Labs having some lasting impact on the research base. The CoE approach is expected to have a more enduring impact on Army-relevant institutional research capacity among funded HBCUs/MIs through investment in organic activity. To help enable this CoE initiative, Ms. Huff led engagement with interested qualifying institutions; drafted the funding announcement in collaboration with topic leads, subject-matter experts, and Army Contracting Command; and conducted extensive outreach to promote the new HBCU/MI funding opportunity.

RESULT

A highly competitive solicitation involving 68 white papers and 21 invited proposals led to three awards to Florida International University (FIU), the University of the District of Columbia (UDC), and the University of Illinois at Chicago (UIC) to be funded for five years at about $450,000 per year for each award. The awards aim to build capacity and expose students to Army research problems in the areas of digital forensics (FIU), environmental modeling and characterization (UDC), and extreme condition chemistry of molecular materials (UIC). The awards thus create the conditions for meaningful growth in HBCU/MI research capability in these areas of high interest to the Army. In the case of the FIU Forensic Investigations Network in Digital Sciences (FINDS) Center, partnership with Grambling State University, Jackson State University, and Florida A&M State University extends this growth throughout the HBCU community. The CoE for Excellence in Acoustic and Seismic Sensing in Urban Environments at the UDC has the additional benefit of HBCU students and faculty working directly with DEVCOM ARL scientists and engineers to understand how acoustic and seismic signals are transmitted through urban environments and how that understanding might influence Army technology development (Figure 1). The EXtreme EnErgy Density CoE at UIC will concentrate resources completely on organic research performance and associated capacity to generate discoveries supporting potential future innovations in explosive power based on novel high-energy-density materials (HEDMs) (Figure 2).

WAY AHEAD

In the past 20 years, the ARO HBCU/MI program has not funded research CoEs of this type. As noted previously, several other approaches have been tried with limited success. The hope is that these centers will establish enduring capability providing diversity in the research ecosystem. With the awards starting in FY21 and being funded for five years through FY25, there is potential to address both the specific scientific questions and the challenges of the HBCU/MI community and the underserved population to increase their STEM awareness and education in areas relevant to the Army. ARO will assess the impact of these CoEs to determine the next investment approach to engage the HBCU/MI community in meaningful research for the Army with the potential to generate a lasting capability. If the three CoEs are successful, they will be well positioned to attract additional research funding from the Army or another DoD component and will continue to produce quality researchers to supply the workforce in direct or indirect support of the Army to sustain vital discovery and innovation.
Army STTR Success Ideas with Impact

The Army Small Business Technology Transfer (STTR) program is an invaluable tool and resource to bring technologies and capability to the Soldier. The Small Business Innovative Research (SBIR) programs (SBIR/STTR) have given the United States of America a strategic innovation and economic growth tool that sets us apart from the rest of the world and assures technological overmatch. The support to small businesses has greatly enhanced the research capabilities of the United States, and helped create innovation centers and new companies stimulating our economy. For over 25 years, ARO has successfully managed the STTR program to transition science and research to the Soldier. Agentase, LLC, TDA Research, Inc., and Tiger Tech Solutions, Inc., include excellent examples of the impact and transition of the STTR program from DEVCOM ARL.

Chemical Warfare Agent Detection

DEVCOM ARL supported Agentase in the STTR program for chemical detectors, and ultimately, the technologies developed, successfully transitioned to a fielded product for the Army and into production with defense prime contractor TeledyneFLIR Corporation. The STTR research originally supported by the ARO Chemical Sciences Program at the University of Pittsburgh demonstrates an excellent example of basic research’s impact from scientific discovery in academia through to a fully fielded military system. The initial basic research of Professor Alan Russell was centered on stabilizing specific enzymes and proteins outside of living organisms in real-world battlefield environments with temperatures ranging from below freezing to over 120 °F. Professor Russell was studying enzymes that could decompose and deactivate toxic compounds, and during that work, discovered a unique way to detect chemical warfare agents. ARO utilized the STTR program, where the academic discovery was transitioned to Agentase, a small business formed to further refine and package the synthetic biology, and develop the product for use on the battlefield.

Originally, there was only a limited number of special users for the chemical detection system and no existing Program of Record for the technology to transition into a fully fielded capability. As the Joint

Figure 1: CIDAS used to find chemical agents.
Program Executive Office for Chemical and Biological Defense (JPEO-CBD) began to observe the progress and capabilities of the new detection system, a new Program of Record, known as the Contamination Indicator/Decontamination Assurance System (CIDAS), was approved to continue testing, evaluation, and development of the system (Figure 1). In parallel to the transition from the University of Pittsburgh to Agentase, the success was recognized within the defense industry, which led to Agentase becoming acquired by TeledyneFLIR. This demonstrates not only the development of a successful new sensor and a new capability for the Soldier, but also the success of the STTR programs to create new businesses that are successfully supporting national security. TeledyneFLIR continues to support working with small businesses to transition their ideas to capabilities for national security.

Cleaning and Decontamination Solutions

In the SBIR/STTR program, TDA has matured many technologies, including from Procter & Gamble and academia, to commercial products used by the military today. In their development of technologies, they have worked with many large companies and defense prime contractors to include TeledyneFLIR and Procter & Gamble. The STTR collaborations led to the commercialization of the detergent SSDX-12® for the cleaning of aircraft and contaminated equipment (Figure 2).

The original STTR research on electrochemical chlorine dioxide (eClO₂) decontamination technology consisted of a battery-powered and -operated sprayer integrated with an electrochemical cell, sodium chlorite, sodium bromide salts, and buffer/additives (Figure 3). The eClO₂ system is registered with the Environmental Protection Agency (reg. # 85797-1) as an effective decontaminant for anthrax spores. During the development process, TDA discovered that decontamination efficacy improved by adding a mixture of commercially available surfactants to the base formulation. More specifically, the surfactant emulsified and rapidly lifted hydrophobic chemicals from military-relevant surfaces without requiring any mechanical agitation. TDA has achieved commercial sales of the surfactant component as a nonreactive detergent solution qualified for use in routine aircraft cleaning per MIL-PRF-87937 and facilities exposed to heavy metals such as aircraft maintenance facilities. TDA is transitioning to expand their SSDX-12® and eClO₂ for commercial and military capabilities by exploring cleaning for removal of other hazardous compounds, skin decontamination, and efficacy against emerging chemical and biological hazards. As a result of their successes within the STTR and SBIR programs, TDA created a private innovation center within their company.

COVID-19 Detector FDA Approved

The startup Tiger Tech has been supported in Army SBIR and STTR programs for the development of a Warfighter performance monitor. When the COVID pandemic started in early 2020, Tiger Tech used technology from the Warfighter Monitor to develop the COVID Plus Monitor. This noninvasive yet powerful tool is the first artificial intelligence/machine learning–based product to receive an Emergency Use Authorization by the Food and Drug Administration (FDA). One of the greatest advantages of the COVID Plus is that it allows users to affordably and quickly assess individuals for COVID-19 risk. In fall 2021, the COVID Plus was used to assure the safety of Soldiers and civilians participating in Project Convergence 21 at White Sands Missile Range, New Mexico (Figure 4). Currently, the COVID Plus is being implemented in the Army and civilian settings across the United States. The STTR and SBIR programs provided the foundational funding for developing this monitor for national health security.

The STTR and SBIR programs have been greatly successful in developing new technologies for the Soldier and commercial markets. The measure of their success has been difficult to quantify except in demonstrating the successful products in the hands of the Soldier. Success in these programs is reliant on dedication to taking the technology to the next level of maturity, and each of the examples outlined here followed a very different path, demonstrating the need to understand the complex nature of bridging the technology “valley of death.”

Figure 2: TDA SSDX-12® aircraft cleaner in use.
Figure 3: TDA eClO₂ on-demand sprayer.
Figure 4: COVID Plus testing at Project Convergence 21, White Sands Missile Range, New Mexico.
SUCCESS STORY

Harvesting Localized Plasmons on Noble Metal Nanostructures for Enhancing Charge Transfer at an Electrochemical Interface

The ARO Electrochemistry Program identified and supported research focused on the successful establishment of protocols for implementing the localized surface plasmon resonance (LSPR) phenomenon and its demonstration of enhanced electrochemical charge transfer for the oxygen evolution reaction (OER). LSPR is when electric fields near the particle’s surface are greatly enhanced and the particle’s optical absorption has a maximum at the plasmon resonant frequency. The OER is a limiting reaction in the process of generating molecular oxygen through chemical reaction, such as the oxidation of water during photosynthesis, and electrolysis of water into oxygen and hydrogen. Developing improved catalysts for the OER is the key to the advancement of a number of renewable energy technologies. This effort successfully demonstrated enhanced OER activity, and the fundamental mechanism of hole injection was studied in the context of that OER mechanism.

CHALLENGE

The key challenge is to understand, at a fundamental level, the nature of hot electrons on the charge transfer processes and how it influences the electrocatalysis. In this case, the principal investigator shows clear evidence of the hole injection enhancing the oxidative process of the OER, which is important to fuel cell applications.

ACTION

In 2018, Dr. Robert Mantz (former Electrochemistry Program Manager) met with Professor Sanjeev
Mukerjee at Northeastern University regarding this research and subsequently received a white paper focused on understanding, at a fundamental level, charge transfer processes at the interface of a plasmonic generator and its consequent electrochemical response. In 2019, Dr. Mantz encouraged Professor Mukerjee to develop this concept into a multi-pronged study to experimentally, computationally, and analytically characterize this phenomenon in the context of quantum-confined nanostructures in conjunction with its ability to effect efficient transfer to both electron and hole carriers; a grant was awarded in 2020. Dr. De Long took over managing the program and Professor Mukerjee’s grant in 2021.

Professor Mukerjee’s progress, summarized here, involves proactive steps taken for the success of this effort to include (1) being awarded a Defense University Research Instrumentation Program (DURIP) grant related to this project, enabling the acquisition of a tip-enhanced Raman surface probe microscope; and (2) successfully implemented a High School & Undergraduate Research Apprenticeship Program (HSAP/URAP) initiative to provide avenues for undergraduate and high school students to remotely analyze electrochemical data with MATLAB-based routines.

RESULT

A key result of this study was a demonstration of the LSPR effect in its ability to enhance charge transfer at an electrochemical interface. For this, a multifaceted approach was invoked to study a well-known OER on semiconducting nickel (Ni) layered double hydroxides (LDHs) with and without iron (Fe) and cobalt (Co) doping. Hence, this investigation targeted LSPR-generated hot electrons having enough energy to cross the Schottky barrier at a noble metal–semiconductor interface (Figure 1a). As shown in Figure 1b, the doping of nickel hydroxide (Ni(OH)₂) with Fe and Co provided very different responses to the corresponding cyclic voltammogram, wherein Co shifts the Ni²⁺/Ni³⁺ redox peaks to the negative of the undoped reference Ni(OH)₂, and in contrast, Fe shows a positive shift. Simultaneous doping of both probes a response in the middle depending on the doping ratio. Clear evidence of plasmonic enhancement of the OER is provided in Figure 1c. This switch to the Ni³⁺ oxidation state is critical for the first abstraction of protons from water required to initiate formation of surface-adsorbed OH* species. Such doping and its consequent effects on the density of states and therefore charge separation of electron and hole pairs were the subject of intensive fundamental studies. It is important to note that this LSPR pairing with a semiconductor is to demonstrate the optimum level of momentum required to transport the hot electron across the junction. As reported in Figure 1d, clear evidence for different bandgaps was determined for LDH Ni(OH)₂ as compared to the Fe- and Co-doped analog. The relatively large bandgap for Ni(OH)₂ (NiLDH) renders it to be nonresponsive to light larger than 250 nm; hence, no direct electron-hole pair can be generated with illumination in the visible and near-infrared bands, thus not favorable for photochemistry without a plasmonic response. For NiFeLDH and NiFeCoLDH, they are responsive to visible light and amenable for electron-hole creation, and hence hole injection for enhancing the OER. Wavelength-dependent photoelectrochemistry experiments conducted on LDH materials exhibited small photocurrents (Figure 2a), as opposed to the reference glassy carbon where negligible photocurrents were detected (540 nm or higher), hence no effect of light on OER activity. However, in NiLDH, comparable contributions were found for all wavelengths indicating the role in

Figure 1: (a) Processes associated with plasmon generation and hot carrier transport across a noble metal–semiconductor junction. (b) Electrochemical response with and without light of 516 nm, 110 mW on various LDH materials (c) AC photocurrent measurements to evaluate plasmonic and non-plasmonic response to light of various wavelengths. (d) Bandgap measurements using diffuse reflectance and Kubelka–Munk transformation.
surface plasmons in enhancing charge injection and separation. On the other hand, NiFeLDH being an indirect bandgap material (2.2 eV) indicates that the photo-response comes from both the plasmonic injections from surface plasmons and those inherent in the material. Detailed Rietveld refinement was carried out on all the LDH materials (Ni, FeNi, and FeCoNi) to facilitate band structure calculations. These are shown in Figure 2b-c using NiFeLDH as a representative example. The results mentioned previously are an effort to establish well-known protocols for such plasmonic-driven charge injection processes. This effort is in the final stages of being reported in terms of how the OER mechanism is driven by hole injection in semiconductors possessing such diverse bandgaps and band structure. This is a striking example of the plasmon-injected resonance electron transfer (PIRET) process.

WAY AHEAD

A firm understanding of such charge transfer mechanisms will greatly improve our ability to design unique composites of LSPR and electrochemically relevant surfaces (metal catalysts or semiconductors). Future efforts will need to focus on gaining an understanding of charge injection in the context of intercalation. Most of the lithium (Li) cathode materials examined by DEVCOM ARL are variants to transition metal LDH structures; hence, whether or not hole injection via LSPR can effect Li charge compensation during its intercalation into these host structures is an open question. Only then will researchers be able to determine to what extent it is possible to enhance detection limits. The exciting prospect of approaching the single molecule detection level via restricted ionic mobility would enhance DEVCOM ARL sensing capabilities (future effort).

SUCCESS STORY

Intelligent Scanning Electrochemical Microscopy

This ARO-funded initiative developed a new visualization method for tracking catalytic activities on surfaces. Visualizing the local chemical reactivity of catalysts in liquid environments is critical for developing new energy generation and storage devices (e.g., fuel cells) that can power land and air vehicles as well as provide personal power to Soldiers. ARO funding enabled development of a new intelligent scanning electrochemical microscope that enabled, for the first time, simultaneous imaging of structure and chemical reactivity of surfaces in the liquid phase.

CHALLENGE

Fuel cells generate electricity quietly and without pollution; therefore, they are a promising technology to provide energy for Soldiers and vehicles. Moreover, electricity generation in fuel cells typically occurs through the oxidation of hydrogen, which can be synthesized from water and electricity through water electrolysis in remote locations. Both fuel cells and water electrolyzers require catalysts. Improved catalysts could be created if scientists could measure key structure–activity relationships of particles while they are operating in the liquid phase. The goal of this work is to develop a microscopy technique that can unequivocally measure these structure–activity relationships. Improvements in the catalyst performance would translate to higher efficiencies and better fuel use in fuel cells and electrolyzers.

ACTION

In 2017, Dr. Robert Mantz (former Electrochemistry and Electrocatalysis Program Manager) received a white paper from Professor Kevin Leonard at the University of Kansas that was focused on investigating surface interrogation scanning electrochemical microscopy (SI-SECM) as a tool for measuring surface-adsorbed intermediates that occur during electrocatalytic reactions. Dr. Mantz encouraged Professor Leonard to develop this concept into a multi-pronged study to experimentally and analytically characterize this phenomenon in the context of measuring catalytic activity and
electrochemical carbon dioxide (CO2) reduction. This would enable the study and development of new catalysts to synthesize liquid fuels from CO2 and water using only renewable electricity, which enhances the ability to scavenge expeditionary power from alternative energy sources as pursued within the DEVCOM ARL Energy Sciences Competency.

Figure 3: Scheme of the tip approach for (A) negative, (B) positive, and (C) mixed feedback effects for intelligent SECM imaging of an Au band on a grooved glass substrate under a disk-shaped platinum (Pt) nanotip with a thin glass sheath. Dashed lines with arrows indicate the tip movement. O and R are the oxidized and reduced forms of a redox mediator, respectively. Intelligent (D) reactivity and (E) topography images, and (F) constant-height image of 2.8-µm-wide Au bands embedded in a grooved glass substrate in 10-mM hexaammineruthenium (Ru(NH3)6)3+ and 1-M potassium chloride (KCl). Each pixel is equivalent to 1 µm × 1 µm. The tip was scanned laterally from the left bottom corner and stepped upward after each line scan. The outer and inner tip radii of 0.44 and 0.28 µm, respectively, were determined by scanning electron microscopy (SEM).

Way Ahead

The research team is now able to utilize this technique to “see the chemistry” at the nanometer scale on functional electrocatalysts designed for fuel cells and electrolyzers. In addition, Dr. Leonard has been in discussion with DEVCOM ARL intramural researchers to enable this technique to study electrochemical carbon dioxide (CO2) reduction. This would enable the study and development of new catalysts to synthesize liquid fuels from CO2 and water using only renewable electricity, which enhances the ability to scavenge expeditionary power from alternative energy sources as pursued within the DEVCOM ARL Energy Sciences Competency.

Figure 4: SEM images of (A) Au bands embedded in a glass substrate, (B) Au band milled by focused ion beam, and (C) cross section surrounded by the dotted line in part (B). (D) AFM image of the non-milled Au band. (E) Final z positions of the tip approach (blue circles) and (F) z positions of the substrate determined by fitting approach curves with theoretical or simulated curves (red circles). Dashed lines represent AFM topography from (D). Dotted lines represent the edge of the Au band.

Way Ahead

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Results

• Led to collaboration between the University of Kansas and University of Pittsburgh on the development of intelligent SECM.

• Developed a new visualization method for tracking catalytic activities on surfaces with the ability to distinguish reactive from inert.

• Determined that measuring these structure–activity relationships allows for improvements in the catalyst performance creating higher efficiencies and better fuel use in fuel cells and electrolyzers.

Anticipated Impact

Fuels cells are a promising technology to provide energy for Soldiers and vehicles, because they generate electricity quietly and without pollution. The microscopy technique developed within this project holds the potential to develop new catalysts to improve the performance of these electrochemical devices.

ARL Competencies:

Energy Sciences
**Program Manager**

**Dr. Elizabeth King-Doonan**

Dr. King-Doonan completed her undergraduate studies at Boston University, receiving her B.S. in Marine Sciences in 2012. She trained as a biogeochemist 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 the Environmental Chemistry Program.

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**Current Scientific Objectives**

1. Achieve understanding of the structure and reactivity of chemicals in multiphase environments, where reactions and transport processes occur between the solid, liquid, and gaseous phases, that, if successful, will mitigate the impact of attacks or natural disasters by enabling accurate assessment of chemical transport and thus rapid response by future Army forces.

2. Develop cutting-edge analytical and experimental approaches to discern compounds of interest in complex environments that, if successful, will enable new capabilities for the detection and source partitioning of biological and chemical threats.

3. Advance computational efforts to predict chemical fate, transport, and transformation over a wide range of temporal and spatial timescales that, if successful, will close critical knowledge gaps that limit relating nanoscale chemical reactions to macroscale environmental dynamics.

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**SUCCESS STORY**

**Biogeochemical Control of Nanoparticle Interfaces**

The ARO Environmental Chemistry Program identified and supported research focused on understanding the link between aqueous biogeochemical compounds and nanoparticle structure and reactivity in complex environments. These insights will enable the Army to reliably predict and control nanoparticle interactions for applications such as contaminant and waste removal, corrosion resistance, and sensing.

**CHALLENGE**

Science and engineering related to nanoscale particles, approximately 1 to 100 nm in size, has the potential to advance military capabilities, from enhancing Soldier survivability to modernizing material for equipment and weapons. The innovative potential of nanotechnology is related to the fact that a material’s properties at the nanoscale—chemical reactivity, fluorescence, electrical and thermal conductivity, and magnetism—differ from the bulk scale as a function of particle size. Thus, working at the nanoscale enables scientists to develop technology with specific and unique physical, chemical, mechanical, and optical properties.

The great advancements enabled by nanotechnology also bring great challenges. One such challenge is understanding the role of the corona in nanoparticle interactions. The corona is the layer of environmental media that adsorbs to a nanoparticle and drastically alters the structure, reactivity, and functioning of its surface (Figure 1). Corona formation is a function of the chemical, biological, and physical properties of both the nanoparticle and the surrounding aqueous environment. While some research has focused on protein corona for biomedical and human toxicity applications, the role of other biomolecules (e.g., metabolites), metals, and natural organic matter on the functioning of nanoparticles is virtually unexplored.

**ACTION**

In 2018, Dr. Robert Mantz (former Environmental Chemistry Program Manager [Acting]) received a white paper from Professor Vicki Grassian at the University of California, San Diego that was focused on understanding how the molecular dynamics at geochemical interfaces control the fate and transport of chemical compounds in soil environments. Dr. Mantz encouraged Professor Grassian to develop this concept into a multi-pronged study to experimentally, computationally, and analytically characterize the transformation of both biological and chemical compounds on geochemical interfaces.
Dr. King-Doonan began managing the Environmental Chemistry Program and Professor Grassian’s grant in 2019. Dr. King-Doonan recognized the potential of this topic to form the fundamental understanding of how military nanotechnology interacts with complex environmental media and met with Professor Grassian to learn about the status of her research. Professor Grassian’s progress highlight the breadth of fundamental knowledge to be gained in nanoscience through the analytical techniques developed in her lab. To advance these techniques further, Dr. King-Doonan encouraged Professor Grassian to apply for a Defense University Research Instrumentation Program (DURIP) grant to advance an emerging technique, coupling Raman spectroscopy and optical infrared microscopy for the direct nanoscale measurement of organic and inorganic compounds involved in interface chemistry and contaminant transformation—a feat that has been previously unattainable. Professor Grassian submitted a successful DURIP proposal that was selected for funding in 2021.

**RESULT**

The objective of Professor Grassian’s project is to determine the key transformations of chemical agents on nanoparticles under variable environmental conditions. Nanomaterials comprising mineral phases such as iron oxides (e.g., hematite and goethite) and titanium dioxide (e.g., anatase and rutile) were selected as model materials because they are ubiquitous in both natural and engineered nanoparticles. In 2021, Professor Grassian and her research team made significant advancements under two focus areas: (1) understanding the transport and transformation of chemical threats on nanomaterial interfaces and (2) concurrently probing the behavior of biological components, oxygen ions, and dissolved organic matter.

For the first focus area, Professor Grassian focused on the interaction between monoethanolamine (MEA)—a diverse compound that is characterized as a toxic surfactant, decontaminant, and potential conduit for carbon dioxide capture—and oxide surfaces. Experiments were performed over a range of solution concentrations and pH, and adsorption was quantified via attenuated total reflectance Fourier transformation infrared spectroscopy (ATR-FTIR). What Professor Grassian discovered was that MEA adsorption mechanisms evolved with changing environmental conditions. At low pH, MEA adsorption onto negatively charged oxide surfaces was low and dominated by hydrogen bonding. As pH increased (pH > 6), MEA–surface interactions became dominated by electrostatic attraction, preferentially concentrating protonated species (Figure 1). Interestingly, these interactions led to the formation of a previously undocumented product that stays adsorbed onto the oxide surface, permanently altering the reactivity of the nanomaterial (Rose et al., in review).

For the second focus area, Professor Grassian and her team focused on the dynamics of competitive adsorption of four common amino acids onto oxide surfaces. They discovered that biomolecules formed extensive multilayer coronas when phosphate nucleotide groups interacted with the oxide interfaces. When non-phosphate functional groups were exposed to the oxide interface first, unstable single-layer coronas formed. Furthermore, when proteins were exposed to oxide interfaces in the presence of mineral phosphate, they exhibited significant changes in their conformational shape, which is a critical driver of protein function (Figure 1; Ustunol et al., 2021). These results indicate that the chemical structure and composition of biomolecules affect the timing and extent of corona formation and vice versa.

**WAY AHEAD**

Professor Grassian will build upon these results in coming years. First, her research team will expand their results related to MEA transformation by identifying the chemical transformation products and kinetics at the oxide interface. These results will provide critical insights into the interaction of aqueous contaminants with filtration nanomaterials that experience rapid degradation/fouling in complex waste streams. Professor Grassian and her team will also explore the adsorption of more complex chemicals onto mineral surfaces by developing new micro-spectroscopic tools to spatially discern adsorbate-surface interactions. By coupling ATR-FTIR with atomic force microscopy-infrared spectroscopy (AFM-IR), Professor Grassian will probe the interactions between chemical species to discern the spatial and temporal extent of adsorbate-surface interactions. Professor Grassian will also leverage her newly awarded DURIP grant to advance an emerging technique, coupling Raman spectroscopy and optical infrared microscopy, to discern reactions between organic compounds and inorganic compounds simultaneously—a goal that has yet to be achieved in the literature.

**Anticipated Impact**

Elucidating the mechanisms driving nanoparticle-biochemical interactions in complex environments is expected to enable future leap-ahead technologies in the areas of field-based sensing, water filtration, and biotechnology.
In 2021, Dr. King-Doonan presented the results from Professor Grassian's project to the scientists and engineers from DEVCOM ARL's Biological and Biotechnology Sciences (BBS) Competency. The BBS Competency aims to develop a better understanding of biological–chemical interactions in military environments to enhance biotechnology precision and control, and focus on future applications of the research. Dr. King-Doonan and Professor Grassian have begun to discuss longer-term research efforts that focus on expanding the understanding of interface chemistry from nanomaterials to other environments of interest, including biofilms and surface films.

SUCCESS STORY
Physiochemical Properties of Biological and Chemical Aerosols

This ARO-funded initiative developed a new technique that can trap single particles for comprehensive characterization and observation of chemical reactions. This unprecedented technique will provide the Army with new strategies by which biological and chemical threats can be monitored, measured, and manipulated.

CHALLENGE

Aerosols, the suspension of liquids or solids in a gaseous matrix, play an important role in a wide range of technical areas including sensing and communications, human health, global climate, and cloud formation. How aerosols interact with their surrounding environmental media depends on a number of parameters intrinsic to both the aerosol and the environmental matrix. These interactions can have far-reaching implications for the stability, toxicity, and transport of biological and chemical threats relevant to the military (e.g., nerve agent detection) and the general population (e.g., the transmission of COVID-19).

Due to the physical and chemical complexity of aerosol particles, and the interdisciplinary nature of the science—often requiring physics, chemistry, biology, and optics—the current knowledge of aerosol fate and transport is incomplete. In fact, most studies focus on understanding bulk-averaged and time- and space-integrated aerosol chemistry, which fails to capture important particle–particle interactions and processes. While strides have been made to capture and characterize single particles in a liquid matrix, significant challenges arise when these techniques are applied to gaseous matrices. Mainly, the capability to stabilize and manipulate a single aerosol particle is lacking, as is the analytical framework to obtain chemical information from a stabilized particle.

ACTION

In 2016, Dr. James Parker (former Environmental Chemistry Program Manager [Acting]) received a white paper from Professor Chuji Wang at Mississippi State University that proposed to overcome the limitations of chemical characterizations of single particles by developing a technique where single particles were trapped using the radiation forces formed in a hollow laser beam. This would enable the particles to be stabilized without the use of other physical forces that would impart their own interactions with the particle. Once stabilized, spectroscopic techniques (e.g., Raman) could be applied to chemically characterize the particle. Dr. Parker recognized the potential impact that this technique could have on the environmental chemistry community and funded the proposal later that year.

In the ensuing years, through site visits and the annual Chemical Sciences Branch’s Basic Research Review, Dr. Parker facilitated an informal collaboration between Professor Wang and Drs. Gorden Videen and Yong-Le Pan from DEVCOM ARL CISD. Drs. Videen and Pan had been familiar with Professor Wang’s research, as he was a rising star in the field of optical chemistry, and they were able to work with him to fine-tune the techniques for aerosol trapping.

When Dr. King-Doonan arrived at ARO in 2019, Professor Wang was in the final year of his effort; Dr. King-Doonan immediately recognized the importance that these analytical capabilities would have on sensing and detection. With over 15 peer-reviewed publications and two journal covers from this three-year effort, it seems the scientific community recognized this as well. In 2020, Dr. King-Doonan kicked off a discussion with Professor Wang and Drs. Videen and Pan about the success of the current effort and potential next steps. With so much left to still discover, the group began to narrow in on the topic of manipulating chemical reactions on the trapped particles. This would enable, for the first time, inducing and measuring simultaneous reactions on a single particle to fully understand the thermodynamics and kinetics of chemical fate, transport, and transformation in the atmosphere. In 2021, following a successful review process, Dr. King-Doonan funded Professor Wang’s effort as a Cooperative Agreement with Drs. Videen and Pan to strengthen the collaborative nature of this effort with DEVCOM ARL CISD and support the DEVCOM ARL BBS and Military Information Sciences (MIS) Competencies.

RESULT

Through his initial effort, Professor Wang developed the universal optical trap (UOT) for single-particle atmospheric aerosols. For the first time, aerosol particles of an arbitrary shape (i.e., irregular) and
ARL Competencies:

Results

- Developed first-of-its-kind UOT-RS system that enables the detection and characterization of any type of airborne particle—natural or deliberately disseminated.
- Measured the distribution of a simulant for the chemical agent VX in an organic aerosol droplet and determined that the evaporation rate increases four times when VX is adsorbed to aerosols.
- Observed, in real time, the formation of protective coatings on bioaerosol particles via the ozonolysis of fatty acids. This mechanism explains why bioaerosols exhibit enhanced retention time and decreased reactivity toward mitigation efforts as they evolve in the environment.

Anticipated Impact

This research is expected to enable contactless particle manipulation and allow for rapid and precise physiochemical characterization. This breakthrough is expected to enable leap-ahead technologies for monitoring a wide range of aerosol particles that affect visibility and communication, as well as Soldier exposure to smoke, diesel exhaust, and chemical, biological, radiological, nuclear, and explosive threats.

WAY AHEAD

In 2021, Professor Wang was awarded a Cooperative Agreement through the Environmental Chemistry Program. Through a formal collaboration, Professor Wang will embark on a new research project with Drs. Videen and Pan of DEVCOM ARL CISD to control and manipulate the chemical evolution of single particles in support of the DEVCOM ARL BBS and MIS Competencies. Through the development of a single-particle reactor, Professor Wang will have the ability to induce chemical reactions on particles stabilized in the UOT. This topic will build on Professor Wang’s previous research by providing, for the first time, capabilities to monitor oxidation, reduction, adsorption, and desorption processes for single particles as a function of a suite of environmental variables including reactant concentration (e.g., OH, O₃, NO₃, and Br), humidity, pH, temperature, and UV radiation.

The focus of this award will be on the chemical evolution of Hg on bioaerosol particles. Hg was selected as a model element given its unconstrained complex cycling in the environment and its potential military relevance as a sensor component, toxic contaminant, and tracer of various industrial activities. Bioaerosol particles were selected as the model substrate given their observed high surface reactivity. Through this effort, Professor Wang and DEVCOM ARL CISD will gain insight into the thermodynamics and kinetics of specific reactions on bioaerosol particles and also develop a novel technique for precisely detecting and characterizing any type of airborne particle.
SUCCESS STORY

Hierarchical Functional Materials via Polymer-Protein Assembly

This ARO initiative led to the development of a novel strategy for effectively interfacing synthetic polymers and biological enzymes that confer protection to the enzymes such that they retain stability and activity in non-biological environments. This effort further demonstrated that this approach could be used to decompose compostable plastics, offering the potential to significantly alleviate waste management issues in austere forward-operating environments.

CHALLENGE

Natural materials, such as proteins, exhibit unique properties and complex functions such as structural control, catalytic activity, molecular transport, and modulated responsiveness. The ability to translate this type of functionality to synthetic non-natural systems would represent a revolutionary advance in the development of dynamic, responsive material systems capable of performing complex functions. Unfortunately, to date, there has been limited success in obtaining hierarchical ordered systems with such functional complexity using solely synthetic materials, and efforts to preserve the structure and functionality of biological materials in non-biological environments have remained elusive.

ACTION

Based on prior research experience in the design and synthesis of polymeric materials for transdermal drug delivery, ARO Polymer Chemistry Program Manager Dr. Poree recognized the potential for polymers to act as “containers” to encapsulate and thus stabilize biological materials in non-natural environments. Through complementary efforts, ARO Biochemistry Program Manager Dr. Stephanie McElhinny was exploring novel strategies in biomolecular self-assembly with a particular interest in innovative approaches for integrating biomolecules with synthetic systems to support biological activity outside the natural biological environment and in nonaqueous conditions. Recognizing this shared vision, the two program managers began to jointly explore how polymeric materials could be rationally designed to effectively co-assemble with biological materials to achieve functional biohybrid materials that combine the complex functional properties of biological materials with the stability and processibility of synthetic polymers. In 2016, Drs. Poree and McElhinny supported a research effort at the University of California, Berkeley to establish the design principles for protein stabilization in non-native environments. More specifically, this effort sought to exploit the statistical...
trends in protein sequence and surface chemistry to develop rationally designed random heteropolymers (RHPs) with similar chemical features and spatial distributions of side chains to match the surface pattern of natural proteins (Figure 1). It was hypothesized that this approach would maximize short-range interactions between the protein and synthetic polymer that would result in the polymer forming a protective shell around the protein while also constraining the protein and thus preventing changes in its structure.

Figure 1: Statistical analysis of protein surfaces enabled the rational design of RHPs as a protein “shell.” These polymers stabilize proteins in a wide variety of solvents. Image courtesy of the Ting Xu Laboratory, University of California, Berkeley.

RESULT

In 2018, the research team demonstrated the successful incorporation of functional proteins into synthetic polymers. To achieve this, the research team performed a computational surface analysis of folded water-soluble proteins and assigned the surface amino acids based on hydrophobicity and charge. Interestingly, this analysis revealed that proteins show characteristic distributions or “patches” of similar hydrophobicity and charge with a typical patch size being 1–2 nm in diameter as well as 1–2 nm in inter-patch distance. The researchers then designed RHPs with similar chemical features and spatial distributions of side chains to match the surface pattern of the modeled proteins. This was done using a reversible deactivation radical polymerization technique that makes it feasible to synthesize heteropolymers with reliable control over the statistical monomer distribution. In this initial study, the RHP and protein (horseradish peroxidase [HRP]) were co-solubilized in water to generate the polymer–protein complexes, and the complexes were studied to determine the feasibility of the polymer to mediate protein stability in toluene, a non-natural organic solvent commonly used for material synthesis and processing. Results revealed that in the presence of the RHP, approximately 80% of the HRP enzyme’s native activity was maintained after suspension in toluene for 24 h, representing several orders of magnitude increase relative to the enzyme without the protective polymer. To demonstrate the generality of the approach, the researchers extended the study to other proteins including green fluorescence protein (GFP) and organophosphorus hydrolase (OPH). OPH was of particular interest due to its excellent ability to degrade organophosphates found in pesticides and chemical warfare agents. In both studies, the RHP was able to protect protein activity in toluene after 24 h (50% activity for GFP, 80% activity for OPH). Furthermore, the researchers were able to demonstrate the feasibility of this approach in the solid state, where the polymer–OPH complex was co-processed with other synthetic polymers, such as polyethylene oxide (PEO) or polycaprolactone (PCL) via electrospinning to render fiber mats. Even in the solid state, these hybrid materials showed retention of OPH activity, and thus organophosphate degradation that persisted for over 90 days (Figure 2). This work thus reveals RHPs as a new strategy for interfacing biological systems with synthetic polymers and could lead to a new class of materials with functions found only in living systems.

Figure 2: Schematic demonstrating the PCL–RHP–OPH fabrication process and material functionality. (a) RHP–OPH co-lyophilized in aqueous solution and re-suspended in toluene formed well-dispersed clusters. (b) RHP–OPH was successfully incorporated inside of electrospun PCL fibers by simply mixing the complex with a PCL/toluene/dichloromethane (DCM) solution and electrospinning the solution. (c) The PCL–RHP–OPH fiber mat retained OPH’s biological activity, converting highly toxic organophosphates (clear liquid) into low-toxicity byproducts (bright yellow liquid). Adapted from DelRe et al. (2018).

ARL Competencies:

- Biological and Biotechnology Sciences
- Sciences of Extreme Materials

Results

- Developed a new strategy for incorporating functional proteins into synthetic polymers, potentially enabling a new class of materials with functions only found in biological systems.
- Demonstrated that these polymer-protein complexes could be designed to act as effective degraders of biodegradable plastics, offering a potentially new route for polymer composting.
- Led to the start-up of a new company called Intropic Materials that will seek to commercially develop these polymer–protein hybrid materials for plastics composting.

Anticipated Impact

If successful, this work will enable a fundamental understanding of the interplay between polymeric materials and proteins to render functional hybrid biomaterials with enhanced stability and activity of proteins in non-biological environments. The resulting biohybrid materials will have a myriad of potential applications of interest to Army including low-energy recycling in austere environments, catalysis, sensing, bioremediation, and even energy harvesting and conversion.
This fiscal year, the researchers demonstrated the RPH approach as a viable strategy for decomposing biodegradable polyester-based plastics, offering a potential route to addressing the current plastics waste challenge (Figure 3). For this study, two biodegradable plastics, polyactic acid (PLA) and PCL, were chosen to show the applicability of the approach. Lipase and proteinase K were selected as the enzymatic proteins due to their ability to cleave ester bonds. The RHP-enzyme complexes were co-processed with either PLA or PCL resin beads such that the RHP-enzyme complexes were embedded throughout the plastic films when manufactured. The results showed that the complexes did not change the character of the plastic, which could still be melted and extruded into fibers like normal polyester plastic at temperatures around 170 °C. To trigger degradation, it was necessary only to add water and a little heat, causing the enzyme to shed the RHP shell and subsequently interact with and degrade the plastic. At room temperature, 80% of the modified PLA fibers degraded entirely within approximately one week, with faster degradation possible at higher temperatures. Under industrial composting conditions, the modified PLA completely degraded within 6 days at 50 °C. Similar results were seen with PCL-based fibers degrading in two days under industrial composting conditions at 40 °C. These results have led to the spin-off of a start-up company called Intropic Materials that will seek to commercially develop these materials.

WAY AHEAD

Going forward, the research team plans to continue to pursue the potential utility of these materials for plastics degradation. Specific plans include developing RHP-protein complexes that can degrade other types of polyester plastics as well as modify the RHP to enable programmed degradation, which could be highly useful for repurposing plastic parts. Concurrently, the team will explore the role of the statistical heterogeneity of radical polymerizations on polymer–protein interactions and how this can be harnessed to maximize the rational design of polymer–protein hybrid materials. Army researchers in the DEVCOM ARL Biological and Biotechnology Sciences competency and DEVCOM Soldier Center have expressed interest in this research. Potential future collaborative efforts will be sought to transition key knowledge products toward the development of novel functional biohybrid materials for applications in food packaging, catalysis, sensing, bioremediation, and low-energy recycling.

SUCCESS STORY

Toward a Novel Single-Molecule Imaging and Manipulation Approach for Rational Polymer Design

This ARO initiative led to a new approach for studying conjugated polymers that made it possible for the first time to measure the individual molecules’ mechanical and kinetic properties during polymerization. The insights gained could lead to more flexible and robust soft electronic materials, such as health monitors and soft robotics.

CHALLENGE

Synthetic polymers are ubiquitous in society, impacting every area of our daily lives from the fabrics in our clothing to the plastics that compose our food and drink packaging, to the composites that make up our automobiles and airplanes. Although the macroscopic properties of polymers are largely determined by the collective properties of polymer molecules, ultimately it is the microstructure and the properties of individual molecules that lay the foundation. Unfortunately, there is always some dispersion, or heterogeneity, in the microstructure of synthetic polymers, making it difficult to precisely determine, predict, or control their resultant properties. As this dispersion/heterogeneity derives from the inherently varied growth kinetics during polymerization, high-resolution techniques that allow for studying polymerization dynamics at the single-polymer level are highly desired.

ACTION

To address this challenge, Dr. Dawanne Poree strategically supported researchers at Cornell University to develop a single-molecule approach for interrogating the growth of individual polymers. As catalytic, chain-growth polymerization is widely used for making synthetic polymers, understanding the kinetics and dynamics of polymerization catalysis was of great interest. In chain-growth polymerization, a polymer chain grows from a catalyst continuously to reach thousands of subunits. The research team proposed a novel approach that combined magnetic tweezer, optical...
Researchers are able to visually observe the wait-and-jump dynamics of the growing polymer. Image courtesy of the Peng Chen Laboratory, Cornell University.

**Figure 4:** Schematic of a magnetic tweezers measurement of a growing polymer (black string) tethered between a surface and a ruthenium-based catalyst that is anchored to a magnetic particle. The catalyst inserts new monomers (blue spheres), leading to the extension lengthening of the polymer. Researchers are able to visually observe the wait-and-jump dynamics of the growing polymer.

**RESULTS**

Using this approach, the research team discovered that individual polymer chains do not grow smoothly and continuously from the catalyst, but rather undergo consecutive “wait-and-jump” steps (Figure 4). With the help of molecular dynamics simulations, the researchers were able to attribute these wait-and-jump dynamics to conformational entanglements formed by newly incorporated monomers. More specifically, during the “wait” period, these polymer tangles, termed hairballs, form around the catalysts as new monomer units are added. The hairballs then randomly unravel, resulting in a “jump” in polymer molecular weight, and a new hairball then starts to form. The researchers also found that the configurations of these entanglements play a key role in determining the polymerization rates and the dispersion among individual polymers, opening new opportunities to manipulate polymer conformation during synthesis to alter their dispersions and thus their properties.

This work, published in *Science*, represented a first-of-its-kind demonstration and received a “Research of the Year” distinction from *Chemical Engineering News* as one of the most notable chemical research advances of 2017.

This fiscal year, the researchers demonstrated that this single-molecule approach could be extended to studying the mechanical and kinetic properties of conjugated polymers during polymerization. Conjugated polymers are of particular interest because of their ability to conduct electrons and absorb light, making them attractive for creating soft optoelectronics, such as wearable electronic devices. However, as flexible as they are, these polymers are difficult to study in bulk because they aggregate and fall out from solution. The single-molecule approach circumvents this issue as only a small amount of polymer is needed, which allows the material to stay soluble in solution. Using the same process described previously, the researchers were able to measure growth of the conjugated polymer, polyacetylene, in real time, and discovered that these polymers add a new monomer per second, a much faster growth rate than their non-conjugated analogs. By pulling and stretching individual conjugated polymers, the researchers were able to assess their rigidity and better understand how they can bend in different directions while remaining conjugated and retaining electron conductivity. They also discovered that the polymers displayed diverse mechanical behaviors from one individual chain to the next—behaviors that had been predicted by theory but never observed experimentally.

**WAY AHEAD**

These recent advances in single-molecule approaches have made it possible to study polymers and polymerization reactions in real time at the single-polymer level, offering a unique opportunity to study synthetic polymers of importance in materials applications. Future work will involve further development of the single-molecule technique to allow for simultaneous imaging of multiple monomers for copolymer sequencing. If successful, this effort will provide an innovative approach for correlating polymer sequence to its macroscopic properties, which is currently a significant challenge. Collaborations will be sought with in-house DEVCOM ARL researchers, particularly within the Polymers Branch, in support of the DEVCOM ARL Sciences of Extreme Materials Competency to potentially use this technique to probe the structure-property relationships of polymers relevant to the Army.
Dr. James Parker completed undergraduate studies at Marquette University, receiving his B.S. in Chemistry in 1993. He worked in industry for one year at the Aldrich Chemical Company as a chemist in the pilot plant. In 1994, he enrolled at the University of Mississippi, where he trained as a physical chemist, studying spectroscopy, chemical reaction dynamics, and molecular electronic structure theory, receiving a Ph.D. in Physical Chemistry in 1999. He was a National Research Council Postdoctoral Fellow at the U.S. Naval Research Laboratory from 2000 to 2001, and from 2002 to 2003, he was a Postdoctoral Fellow at the NASA/Goddard Space Flight Center. As a professor, he taught chemistry at Valdosta State University and was a principal research investigator for atmospheric chemistry at the Midwest Research Institute. Dr. Parker has been serving as a Program Manager at ARO since 2009.

SUCCESS STORY
A COVID Pivot Plus Up SBIR Phase II Supplemental Award for Generation of Medical-Grade Oxygen in Real Time at the Site of Use

In FY21, the Defense Health Agency’s (DHA’s) Small Business Innovation Research (SBIR) program announced a competition for 10 supplemental awards to be made with a focus on alleviating the conditions around the COVID-19 pandemic. Dr. Parker immediately saw an opportunity to develop technology for portable, on-demand generation of medical-grade oxygen. Oxygen therapy is used in treating patients with severe symptoms of COVID-19, and thus oxygen supplies are critical in the care of patients. However, oxygen demand can be so high that hospitals run out of oxygen, and this results in the death of severely affected patients. To alleviate this problem, Dr. Parker worked with Global Research, Inc. (Columbus, Ohio), to set up conditions necessary to award funds from DHA. Upon review of Global’s research proposal, DHA agreed to fund supplemental Phase II research on the development of a portable electrochemical oxygen pump with semipermeable membrane technology for on-demand production of medical-grade oxygen.

CHALLENGE
The main technical challenge to overcome in developing semipermeable membrane oxygen separation technology is in having an electrolyte layer that is uniformly nano-thin (about 100 nm) and gas-tight. The very thin electrolyte layer is necessary so that when the semipermeable membrane is in the working state (Figure 1), there is enough flux of oxygen ions such that the rate of oxygen gas production is on the order of about 3 L/min for a device.
CHAPTER 3  
SUCCESS STORIES

ARL Competencies:

Photonics, Electronics, and Quantum Sciences

ACTION

A program announcement for SBIR supplemental COVID Pivot plus up funding was announced by DHA in FY21. Dr. Parker approached Ms. Nicole Fox, ARO SBIR/STTR Program Manager, and DHA with the idea to nominate Global for an award. A previous SBIR Phase II project by Global was successful in demonstrating the viability of the oxygen separation technology at moderate temperatures.

RESULT

Dr. Parker nominated Global, and the company submitted a proposal. Dr. Parker led the proposal evaluation team that recommended funding. The decision was ultimately up to DHA, and after some deliberation, the agency elected to award a $1M supplement to Global to continue development of the oxygen separation technology. This research is directly relevant to the Nanostructure Surface Interactions and Reactivity thrust of the Reactive Chemical Systems Program. The company is currently working to optimize the fabrication process of the 100-nm-thin electrolyte for an approximate 1-m² surface for device application.

WAY AHEAD

Global plans to make available working prototypes at the end of the COVID Pivot supplemental stage for evaluation by Army and industry. The company will transition the technology to industry via license for production and sales to the U.S. Government, hospitals, and the health care industry.

SUCCESS STORY

Extreme Energy Density (EXEED): An HBCU-MI Center of Excellence

In FY21, the Army Historically Black Colleges and Universities/Minority-Serving Institutions (HBCU/MI) program decided to set up Centers of Excellence. Center topics were solicited at ARO. Dr. Parker decided, in consultation with Dr. Robert Mantz, ARO Chemical Sciences Branch Chief at the time, to write a topic on novel energetic materials (Extreme Energy Density [EXEED]) for the Broad Agency Announcement (BAA) call. The topic was developed solely by Dr. Parker, and then was selected by ARO management for publication in the BAA. One Center of Excellence was awarded for this topic.

CHALLENGE

Novel energetic materials are putative compounds that should have two to five times the power yield of trinitrotoluene (TNT). The compounds exist in theory, but there are no known synthesis methods for making them in a stable form at ambient conditions. An example of a novel energetic material is poly-nitrogen. This material can be formed at ultra-high pressures in which molecular nitrogen undergoes polymerization. However, upon release of pressure and return to ambient conditions, the poly-nitrogen reverts back to its molecular form, making it useless as an energetic material for the military. The general technical challenge is to chemically stabilize such materials so that their meta-stability is transformed into very stable materials such as one finds with many molecular crystals.

RESULTS

- The success of this technology will displace the need to have compressed cylinders of oxygen stored in hospitals. It will also displace the need for having large storage containers of liquid oxygen in or near hospitals. Liquid oxygen is extremely dangerous, since it has potential to contribute to high-intensity fires and explosions under certain circumstances. Compressed cylinders present logistics problems for the military and are hazardous (can transform into a rocket) in cases of accidental dropping. The convenience of portable, on-demand oxygen generation at the point of need is a high-value medical application of the developing technology.

Anticipated Impact

Development of semipermeable membrane oxygen separation technology into portable on-demand generation of oxygen at the point of need will result in diminished logistics burden for the Army at remote field hospitals. The technology will be portable and easy to implement, even using batteries as a power source, and will result in a life-saving medical application for Warfighters injured in remote areas. The technology will also benefit civilian hospitals and patients with severe symptoms of COVID-19.

Figure 1: Conceptual view of a working oxygen separation semipermeable membrane. Image courtesy of Mike Tomsic, Global Research, Inc.
Results

• Expected to profoundly impact Army technologies and capabilities in propulsion and explosives.

• Anticipated to discover of new forms of novel energetic materials with two to five times the power density of TNT.

• Anticipated to provide insights on how to stabilize metastable materials formed at high pressures to ambient conditions.

• Anticipated to result in the design and synthesis of new classes of materials such as EMOFs.

Anticipated Impact

The anticipated impact of the EXCEED Center of Excellence is in the area of novel HEDMs that, if successful, will push next-generation energetic materials into yielding power densities of two to five times that of TNT, giving the U.S. Army and DoD unmatched performance of munitions and propulsion systems.

ACTION

Upon publication of the HBCU/MI Centers of Excellence BAA, Dr. Parker reached out to some principal investigators at HBCU/MI institutions to request white papers. Six white papers were received and evaluated. It was determined that just two proposals would be invited. In consultation with Dr. Mantz, two white papers were selected for invited proposals. A panel of Army experts was assembled by Dr. Parker to evaluate the proposals, with Dr. Parker serving as the panel chair. The panel decided that both proposals were excellent and forwarded both with the recommendation for funding. The Physical Sciences Division Director concurred and sent the recommendation forward. The result was that just one proposal was selected for funding, and the awardee was the University of Illinois Chicago with Professor Russell Hemley as the lead principal investigator. The EXEED Center of Excellence is a planned five-year project involving four co-investigators and will be supported at a financial level of $450,000 per year.

RESULT

The award was made on 8 June 2021. The EXEED Center of Excellence is dedicated to the study of next-generation energetic materials to meet future Army needs. The goals of the Center are to create next-generation energetic materials, with a focus on new high energy density materials (HEDMs), to advance understanding of energetic materials in general, and train the next generation of scientists and engineers for the Army and DoD in the field of energetic materials. EXEED is relevant to the Synthetic Molecular Synthesis thrust of the Reactive Chemical Systems Program.

WAY AHEAD

The research plan for EXEED will thus consist of two parallel components: (1) discovery, synthesis, and recovery of new HEDMs and (2) energetics and reaction dynamics, each composed of separate thrusts. The first component is directed toward discovery, synthesis, and ultimately recovery of new HEDMs formed from simple molecular materials, their alloys, and organic precursor molecules. Figure 2 highlights possible outcomes from employment of high-pressure synthesis methods. The second component will utilize time-resolved, including ultrafast, experimental techniques to study the reaction kinetics, intermediate products, and energy release. Both components will take advantage of new synchrotron radiation and fast laser spectroscopy techniques now available to probe chemical reactions under static and dynamic high pressure and temperature (P-T) conditions as well as the pressure-temperature-time (P-T-t) regimes with dynamic compression. An interesting aspect of some proposed research involves creation of energetic metal–organic frameworks (EMOFs). Metal–organic frameworks are coordination networks consisting of metal ions coordinated to organic ligands to form crystalline structures, often with a periodic network of pores. EMOFs are almost unknown, with one example being reported. EMOFs are expected to display interesting thermal and kinetic properties for high-performance energetic materials. Some expected properties are extreme thermal stability, insensitivity to shock, and high energy and power yields due to inherently excellent chemical kinetics.
BIOCHEMISTRY PROGRAM

Program Manager
Dr. Stephanie McElhinny

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 at Chapel Hill, receiving her Ph.D. in Biochemistry in 2004 and conducted postdoctoral research in biochemistry and yeast genetics at the National Institute of Environmental Health Sciences. She came to ARO in 2009 as the Program Manager for Biochemistry.

Current Scientific Objectives

1. 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.

2. Design self-assembled biomolecular architectures to support functional organization of biological molecules in noncellular contexts that, if successful, are anticipated to lead to on-site manufacturing capabilities and responsive materials.

3. 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.

SUCCESS STORY

Magnetically Sensitive Protein May Enable Bio-Inspired Navigation

This ARO research effort, co-funded by the Office of Naval Research Global (ONR Global) and the Air Force Office of Scientific Research (AFOSR), was the first to demonstrate that a protein in birds' retinas is sensitive to magnetic fields and may be a long-sought sensor for biological navigation. The research team discovered that the protein cryptochrome 4 is sensitive to magnetic fields due to electron transfer reactions triggered by absorption of blue light. This research has significant potential to impact future Army capabilities for the navigation of autonomous or manned vehicles in environments where GPS is unavailable, compromised, or denied.

CHALLENGE

It has been clear since the 1960s that birds have a compass that responds to the direction of the Earth's magnetic field and helps them navigate during their annual migrations. However, it is still uncertain how this compass works. Since the early 1980s, it has been known that the magnetic compass in birds is light-dependent. This research effort tested whether a specific light-sensitive protein, named cryptochrome 4, found in the retina of a night-migratory robin could be the magnetic sensor of the bird's compass. Until this research, no cryptochrome protein from a migratory animal that uses a light-dependent compass had been shown to be magnetically sensitive.

ACTION

Dr. McElhinny identified a scientific opportunity for the Army to explore novel strategies to support biological activity outside the natural, biological environment and in nonaqueous conditions. In support of this goal, she recognized the unique advantages of the cryptochrome 4 protein to serve as an exemplar for translating biomolecular activity to nonbiological environments. The potential of this protein to be activated by magnetic field, rather than the binding of small molecules in aqueous solution, provides an ideal opportunity to explore modulation of biomolecular activity that would be amenable to nonaqueous environments. Dr. McElhinny also recognized the significant potential of this fundamental research to impact future Army capabilities in navigation and partnered with ONR Global and AFOSR to support an international team of experts in magnetoreception to determine if cryptochrome 4 was sensitive to magnetic fields.
RESULT

The team of researchers from the Universities of Oxford and Oldenburg, led by Professor Peter Hore (University of Oxford) employed one-of-a-kind analytical instruments that they designed and assembled specifically to probe the magnetic sensitivity of protein molecules. The team developed Broadband Cavity Enhanced Absorption Spectroscopy (Figure 1) and Cavity Ring-Down Spectroscopy approaches that are unique to Oxford and are one of the reasons why the research team is so far ahead of the rest of the world in studying the magnetic sensitivity of cryptochrome proteins. Although these analytical techniques, and others like them, are relatively commonplace in the gas phase, their application in condensed liquid and solid phases (with vastly increased scattering, for example) has been comparatively slow. The research team had to uncover optimal ways to conduct these experiments for aqueous solutions of cryptochrome proteins.

Using these unique analytical capabilities, the research team discovered that cryptochrome 4 is sensitive to a magnetic field and learned that this magnetic sensitivity depends on the ability of the protein to transfer electrons along a specific part of the protein chain. Proteins are chains of amino acids, akin to beads on a string. In cryptochrome 4, the research team found that four of these amino acids in the chain pass electrons from one to the next (Figure 2). Light initiates the electron-hopping process, and this electron hopping then changes the cryptochrome protein in a way that makes it sensitive to magnetic field. If the researchers interrupt the electron hopping by changing the type of amino acids in that series of four, the protein was no longer sensitive to magnetic field. The team also demonstrated that the cryptochrome protein from the migratory robin was much more sensitive to magnetic field than cryptochrome proteins from nonmigratory birds that do not need to navigate. This research was the first to show that a cryptochrome protein from a migratory animal that uses a light-dependent compass is magnetically sensitive. Thus, it is very likely that this protein is a key player in the light-dependent magnetic compass.

WAY AHEAD

More research is required to understand how the magnetic compass works in the bird’s eye. In the bird’s retina, it is likely that the cryptochrome proteins are aligned in an ordered fashion, which could increase their sensitivity to the weak magnetic field of Earth. In addition, there are likely other proteins that work together with cryptochrome to translate the signal received from the magnetic field into signals that are understood by the migrating birds. The research team is currently searching for these unknown interaction partners.

With respect to future applications, this research provides a foundation toward an interesting possible alternative technology for navigation that would only rely on the magnetic field of Earth, unaffected by weather or light levels. The research demonstrated that the magnetic field modifies the cryptochrome protein in a measurable way; thus, a future navigation device could decode detectable changes in the cryptochrome protein to indicate the strength and direction of the magnetic field, which would identify the navigational position on Earth. Rather than using the cryptochrome protein itself in a future device, it is also possible that more robust materials like organic semiconductors could be used, if they were designed to mimic the electron-hopping reactions necessary for cryptochrome’s magnetic sensitivity. A significant amount of research would need to be done before we could get to the point of an actual device based on the bird’s magnetic compass, but this discovery is an exciting first step in that direction.

Results

• Demonstrated that a protein in birds’ retinas is sensitive to magnetic fields and may be a long-sought sensor for biological navigation.

• Discovered that an electron-hopping mechanism along a chain of four amino acids leads to the magnetic sensitivity of cryptochrome 4 protein.

Anticipated Impact

If successful, this work will enable fundamental understanding of the biomolecular mechanisms underpinning magnetoreception in migratory birds, which would have significant potential to impact future Army capabilities for the navigation of autonomous or manned vehicles in environments where GPS is unavailable, compromised, or denied.
SUCCESS STORY

Hierarchical Functional Materials via Polymer-Protein Assembly

This ARO initiative led to the development of a novel strategy for effectively interfacing synthetic polymers and biological enzymes that confer protection to the enzymes such that they retain stability and activity in nonbiological environments. This effort further demonstrated that this approach could be used to decompose compostable plastics, offering the potential to significantly alleviate waste management issues in austere forward-operating environments.

CHALLENGE

Natural materials, such as proteins, exhibit unique properties and complex functions, including structural control, catalytic activity, molecular transport, and modulated responsiveness. The ability to translate this type of functionality to synthetic, nonnatural systems would represent a revolutionary advance in the development of dynamic, responsive material systems capable of performing complex functions. Unfortunately, to date there has been limited success in obtaining hierarchical ordered systems with such functional complexity using solely synthetic materials, and efforts to preserve the structure and functionality of biological materials in nonbiological environments have remained elusive.

ACTION

Dr. McElhinny, the ARO Biochemistry Program Manager, identified a scientific opportunity for the Army to explore novel strategies in biomolecular self-assembly, with a particular interest in innovative approaches for integrating biomolecules with synthetic systems to support biological activity outside the natural, biological environment and in nonaqueous conditions. Through complementary efforts, and based on prior research experience in the design and synthesis of polymeric materials for transdermal drug delivery, ARO Polymer Chemistry Program Manager Dr. Dawanne Poree recognized the potential for polymers to act as “containers” to encapsulate and thus stabilize biological materials in nonnatural environments. Recognizing this shared vision, the two program managers began to jointly explore how polymeric materials could be rationally designed to effectively co-assemble with biological materials to achieve functional biohybrid materials that combine the complex functional properties of biological materials with the stability and processibility of synthetic polymers.

RESULT

In 2018, the research team demonstrated the successful incorporation of functional proteins into synthetic polymers. To achieve this, the team performed a computational surface analysis of folded water-soluble proteins and assigned the surface amino acids based on hydrophobicity and charge. Interestingly, this analysis revealed that proteins show characteristic distributions or “patches” of similar hydrophobicity and charge with a typical patch size being 1–2 nm in diameter as well as 1–2 nm in inter-patch distance. The researchers then designed RHPs with similar chemical features and spatial distributions of side chains to match the surface pattern of natural proteins (Figure 3). It was hypothesized that this approach would maximize short-range interactions between the protein and synthetic polymer, which would result in the polymer forming a protective shell around the protein while also constraining the protein and thus preventing changes in its structure.

**Figure 3:** Statistical analysis of protein surfaces enabled the rational design of RHPs as a protein “shell.” These polymers stabilize proteins in a wide variety of solvents. Image courtesy of the Ting Xu Laboratory, University of California, Berkeley.

This success was made possible by:

Dr. Stephanie McElhinny, Life Sciences Branch

Dr. Dawanne Poree, Chemical Sciences Branch

Citations:


ARL Competencies:

Biological and Biotechnology Sciences
Sciences of Extreme Materials

Results

• Developed a new strategy for incorporating functional proteins into synthetic polymers, potentially enabling a new class of materials with functions only found in biological systems.

• Demonstrated that these polymer–protein complexes could be designed to act as effective degraders of biodegradable plastics, offering a potentially new route for polymer composting.

• Led to the start-up of a new company called Intropic Materials that will seek to commercially develop these polymer–protein hybrid materials for plastics composting.

Anticipated Impact

If successful, this work will enable a fundamental understanding of the interplay between polymeric materials and proteins to render functional hybrid biomaterials with enhanced stability and activity of proteins in nonbiological environments. The resulting biohybrid materials will have a myriad of potential applications of interest to the Army, including low-energy recycling in austere environments, catalysis, sensing, bioremediation, and even energy harvesting and conversion.

This fiscal year, the researchers demonstrated the RPH approach as a viable strategy for decomposing biodegradable polyester-based plastics, offering a potential route to addressing the current plastics waste challenge (Figure 5). For this study, two biodegradable plastics, polyactic acid (PLA) and PCL, were chosen to show the applicability of the approach. Lipase and proteinase K were selected as the enzymatic proteins due to their ability to cleave ester bonds. The RHP-enzyme complexes were co-processed with either PLA or PCL resin beads such that the RHP-enzyme complexes were embedded throughout the plastic films when manufactured. The results showed that the complexes did not change the character of the plastic, which could still be melted and extruded into fibers like normal polyester plastic at temperatures around 170 °C. To trigger degradation, it was necessary only to add water and a little heat, causing the enzyme to shed the RHP shell and subsequently interact with and degrade the plastic. At room temperature, 80% of the modified PLA fibers degraded entirely within approximately 1 week, with faster degradation possible at higher temperatures. Under industrial composting conditions, the modified PLA completely degraded within 6 days at 50 °C. Similar results were seen with PCL-based fibers degrading in 2 days under industrial composting conditions at 40 °C. These results have led to the spin-off of a start-up company called Intropic Materials that will seek to commercially develop these materials.

WAY AHEAD

The research team plans to continue to pursue the potential utility of these materials for plastics degradation. Specific plans include developing RHP-protein complexes that can degrade other types of polyester plastics as well as modifying the RHP to enable programmed degradation, which could be highly useful for repurposing plastic parts. Concurrently, the team will explore the role of the statistical heterogeneity of radical polymerizations on polymer–protein interactions and how this can be harnessed to maximize the rational design of polymer-protein hybrid materials. Army researchers in the DEVCOM ARL Biological and Biotechnology Sciences Competency and DEVCOM Soldier Center have expressed interest in this research. Potential future collaborative efforts will be sought to transition key knowledge products toward the development of novel functional biohybrid materials for applications in food packaging, catalysis, sensing, bioremediation, and low-energy recycling.
Current Scientific Objectives

1. Determine how to prevent, mitigate, and reverse damage to nuclear and mitochondrial DNA and mitochondrial organelles that, if successful, will reduce Warfighter mortality.

2. Determine how to induce selective replication of DNA molecules that have retained their integrity in organelles that, if successful, will improve Warfighter performance and health.

3. Determine how to efficiently exploit the regulatory pathways and protein function revealed by genetic variation (including single nucleotide polymorphisms as well as large-scale rearrangements) that, if successful, will improve Warfighter protection, reduce Warfighter mortality, and dramatically improve physical and cognitive capabilities.

SUCCESS STORY

p53 Overexpression Induces the Formation of Stable Prion Aggregates

p53, an important tumor-suppressor protein, is one of the most well-studied proteins. Over 280,000 papers have been published detailing p53 regulation and function. As such, one might think that everything worth discovering about p53 is already known. This assumption would be wrong. Work done this year by ARO-funded investigator Professor Sue Liebman (University of Nevada) demonstrated that p53 overexpression in the yeast Saccharomyces cerevisiae induces the formation of stable p53 prion aggregates and that these aggregates are stably transmitted through at least 100 generations.

CHALLENGE

The word prion is derived from "proteinaceous infectious particle" and prions are unique in being able to propagate their misfolded state onto normal variants of the same proteins. Prions can rapidly induce other molecules of the same protein to adopt the misfolded prion state, resulting in an exponential increase in prion formation, which then goes on to infect proteins in other cells. All other infectious agents, including viruses, bacteria, fungi, and protozoa, contain either DNA or RNA, or both. Prions are the cause of untreatable and fatal diseases in humans as well as in sheep, deer, and cattle (Figure 1). Prion aggregates have also been implicated in neurodegenerative diseases such as Alzheimer’s and Parkinson’s. The economic cost of prion disease in cattle alone in the United States is around $10B.

Prions are particularly challenging to work with for a number of reasons. Work on mammalian prions must be done in very secure facilities, as prion effects on humans are untreatable and manifest as spongiform neurodegeneration, followed by death. Proteins in the misfolded prion shape have the same sequence as their properly folded counterparts, and thus cannot be treated with antibodies.

Citations:

Results

- Provided key insight into the pathways of prion formation, which is the cause of untreatable, fatal diseases in humans.
- Induced stable prions in S. cerevisiae that were transmitted to offspring for over 100 generations.
- Demonstrated that the cytoplasmic transfer from infected cells induced prion formation in naïve cells.
- Demonstrated the formation of reversible protein aggregations after exposure to stress from ethanol, heat, or starvation.

Anticipated Impact

This work represents a significant step forward to understanding prion biology and ultimately using this knowledge to protect U.S. civilians, Warfighters, and the U.S. economy against the pernicious effects of prions.

ACTION

Dr. Strand, the ARO Genetics Program Manager, identified a scientific opportunity for the Army to explore prion biology using human p53 in the smaller eukaryote Saccharomyces cerevisiae.

Professor Liebman’s team at the University of Nevada first created a strain of S. cerevisiae, which expressed the human p53 gene with an inducible promoter, and then constructed a reporter system to enable the investigators to rapidly identify and visualize cells that had reduced p53 activity due to prion formation.

RESULTS

The team demonstrated that these prions were stable and were transmitted to offspring for over 100 generations. They also demonstrated that the transfer of cytoplasm-induced prion formation in naïve cells (i.e., prion induction does not require the transfer of any genetic material). They then went on to demonstrate that reversible protein aggregation could be induced by subjecting the cells to ethanol, heat, or starvation stress. This work demonstrates that wild-type p53 expressed in S. cerevisiae forms both stable and reversible stress-induced aggregates, and that p53 can seed protein aggregation and prion formation in proteins that do not have an identical amino acid sequence.

WAY AHEAD

Although S. cerevisiae cells are biochemically quite similar to H. sapiens cells, there are differences in the protein chaperones. Further work needs to be done to translate the results of this work to larger eukaryotes. This work represents a significant step forward to understanding prion biology and ultimately using this knowledge to protect U.S. civilians, Soldiers, and the U.S. economy against the persistent and insidious effects of prions.

SUCCESS STORY

Iodide Redistribution is an Evolutionarily Conserved Response to Severe Stress

This ARO initiative led to the development of a novel strategy for mitigating the effects of severe biological challenges such as stroke, traumatic injury, and viral infections on Warfighter health and performance.
CHAPTER 3  
SUCCESS STORIES

ARL Competencies:

Biological and Biotechnology Sciences
Humans in Complex Systems

Results

• Provided key insight into the mechanism of iodide in hyperinflammation and immunosuppression.

• Demonstrated that iodide in the plasma of trauma patients increases 17-fold, of sepsis patients increases 26-fold, and of small mammals increases 3-fold, compared to controls.

• Demonstrated that the redistribution of iodide in response to stress is evolutionarily conserved across species.

• Demonstrated that elevated levels of iodide improve the outcome after severe injury in M. musculus.

Anticipated Impact

An estimated two billion people suffer from iodide deficiency, which can lead to goiter and cognitive impairment. Dr. Roth’s work demonstrates that iodide redistribution is an evolutionarily conserved response to severe stress, that the levels of iodide in human plasma can be significantly increased safely, and that doing so improves the outcome after a severe injury. Clinical trials are underway to validate these findings. If successful, these results will warrant changes in the standard of care after severe trauma, and are expected to significantly reduce injury and mortality in civilians and the future Soldier.

**CHALLENGE**

Severe trauma that stops blood flow to an organ or limb results in major intracellular damage very quickly via ischemia. When blood flow stops, whether from trauma or stroke, it must be restored within minutes or major permanent damage occurs. Restoration of blood flow stops the ischemic damage, but initiates a period of excessive inflammation and hyper immune response, followed by immune suppression. Both hyperinflammation and immunosuppression are dangerous for humans and can lead to death. The challenge is to control and limit hyperinflammation and immunosuppression to reduce Warfighter injury and mortality.

**ACTION**

Dr. Strand and Dr. Marti Jett (U.S. Army Medical Research and Development Command) identified a scientific opportunity and worked together to initiate Army funding to enable this research.

**RESULTS**

The team of investigators, led by Dr. Mark Roth at the Fred Hutchinson Cancer Research Center, measured plasma levels of iodide and determined that they increased 17-fold in trauma patients and 26-fold in sepsis patients, compared to healthy controls (Figure 2). They also measured plasma levels in hibernating ground squirrels, which exhibited a three-fold increase. These results indicate that this is an evolutionarily conserved fundamental response to trauma. They further investigated and demonstrated that elevated levels of iodide are safe and improve the outcome after severe trauma.

**WAY AHEAD**

Dr. Roth launched a company to transition the results of this basic research to clinical use. This company obtained venture capital funding to carry this work forward into human clinical trials. A 14-country, 2,300-patient Phase 3 clinical trial was initiated in November 2021 and is expected to finish by November 2024. Further work is also needed to determine whether Warfighters and civilians are consuming optimal levels of iodide.

“*You should never underestimate the capabilities of the most badass protein polymers on the planet.*”


**Figure 2:** Blood iodide increases in sepsis and trauma patients. Black dots represent plasma iodide values from healthy nonmedical volunteers, n = 208, mean = 5.7 ng/mL, SD = 4.1, SEM = 0.28, range = 0.80–23 ng/mL; blue dots are trauma plasma iodide values, n = 19, mean = 99 ng/mL, SD = 147, SEM = 34, range = 1.2–504 ng/mL; red dots are sepsis, n = 86, mean = 146 ng/mL, SD = 130, SEM = 14, range = 4.3–706 ng/mL. A t test comparing Healthy and Trauma using Welch’s correction for unequal variance, p = 0.0063, and a t test comparing Healthy and Sepsis using Welch’s correction for unequal variance, p < 0.0001. Image courtesy of the Mark Roth Laboratory, Fred Hutchinson Cancer Research Center.
**MICROBIOLOGY PROGRAM**

**Program Manager**

Dr. Robert Kokoska

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 Biochemistry Program Manager, has served as the University Affiliated Research Center Program Manager, and has been the Microbiology Program Manager since 2014.

**Current Scientific Objectives**

1. Discover the dynamics and communication mechanisms that drive robustness and function within bacterial communities that, if successful, will lead to the effective design of microbial-based platforms for on-demand fielded material synthesis.

2. 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.

3. Identify and characterize microbial metabolic programming under harsh environmental conditions that, if successful, will provide new approaches in the field of synthetic biology toward fielded living material systems.

**SUCCESS STORY**

**The Needle in the Haystack: Single Gut Microbe Linked to Cognitive Impairment**

This study identified a single microorganism out of hundreds present in the mammalian gut that can impair cognitive behavior in mice under conditions of physical stress and a diet depleted in carbohydrates. This finding will help the Army form new strategies for developing improved dietary regimens for the Warfighter in order to maintain vigilance within challenging environments.

**CHALLENGE**

There has been a growing appreciation for how the community of microorganisms that inhabit the human gastrointestinal (GI) tract, termed the gut microbiome, affect not only the health of an individual's GI tract but also the behavior, brain function, and cognitive capacity of an individual. Furthermore, diet and the challenging presence of physical or mental stress affect the ability of “healthy microbes” to flourish in the gut. Studies of the “gut–brain axis” include the ability to decipher which microbes within a community produce the metabolites that determine cognitive capacity. The vast complexity of the gut microbiome, which is composed of hundreds of individual microbial species, and the entangled metabolic interactions among these species present a great challenge toward understanding the effects of the gut microbiome on cognition as a function of dietary input and stress. Indeed, microbiome complexity is a major barrier toward fully understanding causation within any complex environmental microbiome, including those found in soils, aquatic environments, or within biofilms.

In approaching this challenge, can one simplify community complexity to an experimentally tractable level so that causation can be understood from a few select microbes within the community? What are the tools and approaches that enable this capability?

**ACTION**

In 2015, Dr. Kokoska and Dr. Frederick Gregory, ARO’s Program Manager for Neurophysiology of Cognition, recognized the vast scientific opportunity in the study of the gut–brain axis for the Army.
They met with scientists from DEVCOM Soldier Center (SC), the U.S. Army Institute of Environmental Medicine (USARIEM), and the Office of Naval Research to discuss an idea for a Multidisciplinary University Research Initiative (MURI) topic that addressed the complexity of this system. From these discussions, the group recognized that a major challenge not addressed within the scientific community was the development of experimental plans and systems that went beyond correlative relationships between components of the gut–brain axis to studies that addressed mechanistic causative relationships. These discussions provided the basis for the development of a successful FY17 MURI topic on the coordinated use of experimentation and multiscale modeling to derive causative links between components of the gut–brain axis.

As part of this MURI, Professor Elaine Hsiao of the University of California, Los Angeles (UCLA; the lead MURI principal investigator) and Professor Rustem Ismagilov of the California Institute of Technology (Caltech) discovered that the combination of a ketogenic diet (one lacking in carbohydrates) and a hypoxic environment (where oxygen is at lower than normal levels, such as at high altitudes) resulted in significant levels of cognitive impairment in mice. These stressful conditions also resulted in a shift in the composition of the gut microbiome. When examining the abundance of rare gut microbial species, the taxa Bilophila stood out as a bacterium that was present in measurable amounts in stressed mice compared to non-stressed controls (Figure 1, top). Following up from this observation, the team discovered that with mice fed a standard diet, the presence of Bilophila alone in the gut was sufficient to impair cognitive behavior (Figure 1, middle and bottom). As the activity of the gut–brain axis includes elements of the immune system and brain function, this group also demonstrated that Bilophila is responsible for immune responses that promote inflammation and irregularities in hippocampal function. Taken together, these findings identify one specific microbial species implicated in physiological dysfunction under conditions of physical stress and a specific dietary input that pointed to the various regulatory nodes of the gut–brain axis. More broadly, this controlled study illustrates an example of how rational reduction of microbiome complexity provides reliable clues toward causative effects between microbial activity and host physiological function.

RESULT

This exciting result was published in the September 8, 2021, edition of Cell Host & Microbe. The gut–brain axis operates as an interconnected bidirectional relay between gut microbes, microbial metabolites, the enteric nervous system (ENS), the immune system, and brain function (Figure 2). This MURI provides informative data toward development of a model that mathematically describes the dynamics and interplay between the various nodes of this complex physiological system. With additional microbiome, ENS, and immune and brain function data, further model refinement will enable a predictive framework for ascertaining the effects of various environmental inputs, such as changes in diet, different stressors, degree of stress on physiological function, and ultimately on behavioral phenotypes. This capability will provide new insights toward the development of reliable dietary regimens tailored toward shaping the gut microbiome in a way that provides optimal human performance in the presence of various physical, mental, and environmental stressors.
WAY AHEAD

There are a number of Army and DoD labs that have great interest in this study and the broader goals of this MURI. The approaches, results, and follow-up studies from this MURI feed directly into DEVCOM SC’s own research goals in the study of the human gut microbiome toward understanding and developing dietary supplements to enhance Soldier performance. The MURI helps inform high-altitude performance studies worked through USARIEM. The detailed studies of the activity and metabolic output of the gut microbiome developed through the MURI directly impact DEVCOM ARL’s metabolic modeling initiatives under the Biological and Biotechnological Sciences and Humans in Complex Systems Competencies. Broadly, this MURI has gained significant exposure throughout the DoD through the DoD-chartered Tri-Service Microbiome Consortium (TSMC), which serves to coordinate intramural and extramural research efforts that advance microbiome research for the benefit of the Warfighter.

SUCCESS STORY

Measuring Gene Expression at the Single-Cell Level: Mapping the Spatial Landscape of a Biofilm

This finding provides the ability to observe patterns of gene expression at the single-cell level across the millions of cells that compose a biofilm and to do so without disrupting the collective spatial arrangement of the cells. This capability will impact the Army’s ability to deter harmful biofilm growth and to engineer constructive biofilms that can either form protective coatings or function as modules for synthesis of valued chemical products and biomaterials.

CHALLENGE

Many microorganisms exhibit the impressive ability to sustain their viability under a broad range of environmental conditions. These conditions include differences in oxygen level, nutrient concentrations and temperatures and the presence of antibiotics, near-toxic levels of metals, and ionizing radiation. The most direct means for understanding how a collective culture of microorganisms maintains its viability under any environmental condition is to examine the expression levels of the many genes that are encoded by a microbe. To date, measurement and analysis of gene expression within a microbial community have been limited to obtaining average gene expression values from all of the cells that make up the community. However, microenvironments exist within a culture that can present noticeable differences in environmental conditions among the various cells within a population and hence result in significant differences in gene expression between individual cells. This is especially true of biofilm communities, which exist in a fixed 3D order and where the local single-cell level environmental conditions are a function of the cell’s location in the biofilm. Beyond that, these conditions are dynamic: they can change over time as the biofilm grows.

In addressing the heterogeneity in gene expression among a biofilm population, the primary challenge is to develop a technique that can interrogate gene expression at a single-cell level while preserving the 3D order of the biofilm and to do so for a broad range of marker genes.

ACTION

At the 2015 annual meeting of the American Society for Microbiology, Dr. Kokoska attended a plenary lecture given by Professor Dianne Newman of Caltech focused on the physiology of the pathogen Pseudomonas aeruginosa and the characteristics of biofilms composed of this microbe. While much of the lecture discussed medical concerns (P. aeruginosa biofilms are present in the lungs of patients afflicted with cystic fibrosis), most of the discussion centered on molecular-level fundamentals—namely, on the role of phenazines, redox-active molecules produced by P. aeruginosa in biofilm development and survival.

Later during that conference, Dr. Kokoska met with Professor Steve Finkel of the University of Southern California, who at that time was funded by the ARO Microbiology Program, where they discussed the intriguing findings from Professor Newman’s lecture. During these discussions, it was noted that the research from Caltech’s Newman Lab fit in well with the research thrust focused on Microbial Community Structure and Function within the ARO Microbiology Program. As Professors Finkel and Newman are colleagues, an introduction was made between Professor Newman and Dr. Kokoska to discuss new hypotheses on how phenazines mediate extracellular electron transfer (EET) through P. aeruginosa biofilms. This led to the development and award of an ARO Single Investigator proposal to Professor Newman in 2016 to explore phenazine-mediated EET and its impact on the metabolic activity of the biofilm microbes and community organization of the biofilm. A number of novel findings resulted from this award, including the role of phenazines bound to extracellular DNA present in the biofilm matrix in promoting EET, which was published in Cell in 2020. Taking these findings a step...
further toward a broader understanding of *P. aeruginosa* biofilm structure and function, two separate but linked events contributed to the capability of determining differences in gene expression among cells in a biofilm population. First, Professor Newman was awarded a Defense University Research Instrumentation Program (DURIP) grant from ARO in 2018 toward the purchase of a wide-field fluorescence microscope, which enables the Newman Lab to perform high-resolution studies of biofilm structure and quantitative studies of the molecular determinants that drive biofilm function. Second, the Newman Lab, in collaboration with Professor Long Cai’s lab at Caltech, developed a technique called par-seqFISH (parallel and sequential fluorescence in situ hybridization), where different fluorescent probes that hybridize to specific mRNAs present in a cell are sequentially applied to a microbial sample. Using the fluorescence microscope purchased through the DURIP award, the team was able to visualize different colored spots within a microbial sample, enabling them to determine differences in expression of many specific genes among the cells in the sample (Figure 3) and, in parallel, a number of different growth conditions (par-seqFISH). When applied to a biofilm, based on distinct microenvironments within a biofilm, one can literally map spatial patterns of gene expression across a biofilm “map” (Figure 4) over time as the biofilm grows. This unprecedented capability illustrates how spatial context is important in providing new insights into the environmental and cellular factors that determine growth and maintenance of a biofilm.

**RESULT**

This creative and powerful technique and its application toward understanding the physiology of biofilms of *P. aeruginosa* was published in *Science* in August 2021. In recognizing that every cell among the millions in a biofilm is exposed to different local environmental conditions, these techniques and the use of fluorescence microscopy to view gene expression at the single cell level will change the way we study and understand biofilms. This study demonstrates activation of different families of genes depending on their location in the biofilm, which can provide insights into how the biofilm functions as a community. For example, certain biofilm regions that are stressed by either a lack of oxygen or specific nutrients will activate genes that are known to promote metabolism in response to that stress. Knowing the spatial “map” of these regions can lead to new hypotheses regarding cellular states in a biofilm, biofilm evolution, and how neighboring regions of a biofilm can share metabolites to help promote survival of the more stressed regions.

**WAY AHEAD**

Through the DEVCOM ARL Biotechnology Branch, the TRANSFORME Essential Research Program, and more broadly through the DEVCOM ARL Biological and Biotechnological Sciences Competency, this capability can provide a new means of studying biofilm formation and the development of strategies that can deter harmful biofilm growth on military materiel. By understanding local biofilm metabolism both spatially and over time, this capability can potentially identify those spatial regions and points of biofilm development that may be most vulnerable to chemical agents that can inhibit either the microbial-based enzymatic activity responsible for material degradation or the microbial interactions within a biofilm necessary for synthesizing these enzymes. This capability can also help guide the engineering of protective biofilms and even the design of biofilms that have the capacity to perform directed biosynthesis or function as environmental sensors or sentinels.

**Disclosures**

This research was made possible through collaboration with the Long Cai’s lab at Caltech and the support of the Defense University Research Instrumentation Program (DURIP) grant from ARO in 2018 toward the purchase of a wide-field fluorescence microscope. It also received support from the ARL Biotechnology Branch, the TRANSFORME Essential Research Program, and the ARL Competencies:

- Biological and Biotechnology Sciences
- Energy Sciences

**Results**

- Published in the prestigious journal *Science* in 2021.
- Discovered and demonstrated a revolutionary high-resolution approach toward studying biofilm physiology that in the long term can also help guide the engineering of biofilms for Army-relevant applications.

**Anticipated Impact**

The ability to track differences in gene expression between individual cells within a biofilm provides the Army with new routes toward controlling and eradicating harmful biofilm growth on Army materiel and a means toward assembling and controlling microbial communities as a platform to synthesize novel biomaterials.
**NEUROPHYSIOLOGY OF COGNITION PROGRAM**

**Program Manager**
Dr. Frederick D. Gregory

**Extramural Lead for ARL Humans in Complex Systems Competency**

Dr. Gregory completed undergraduate studies at Morehouse College, receiving a B.S. in Biology in 1999 and went on to earn his Ph.D. in Neurobiology at the University of California, Los Angeles in 2006. He completed postdoctoral fellowship research under the National Institute of Drug Abuse at Emory University and through the National Institutes of Health’s Institutional Research and Academic Career Development Award at Emory and the University of Iowa.

Dr. Gregory came to ARO in 2012 and then took on the additional role of International Program Manager for Human Dimension from 2016–2021. He currently serves as the Extramural Lead for the Humans in Complex Systems research competency in addition to his role as Program Manager.

**Current Scientific Objectives**

1. Map, measure, and model structural and functional components of multisensory neural processes that, if successful, are anticipated to reveal the capability to modulate human multisensory information processing beyond normal limits and enable seamless bidirectional communication between Soldier’s and intelligent agents in multi-domain training and operations.

2. Determine how brains structure, process, and refine biological neural networks to generate efficient decisions and behaviors, and show robustness to injury that, if successful, will enable a deep understanding of multiscale neural phenomena with potential applications for maintaining peak cognitive performance and ensuring mitigation of injury or environmental stressors for extended periods to effectively limit cognitive fatigue.

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**SUCCESS STORY**

**Expert Camouflage-Breakers Accurately Detect Target in Less than a Second**

In just one-twentieth of a second, experts trained in a new camouflage-breaking technique were able to accurately detect that something is hidden in a scene and precisely identify the camouflaged target. This skillset could mean the difference between life and death.

**CHALLENGE**

In 2011, after a decade of operations in Iraq and Afghanistan, Army helicopter pilots were continuing to crash due to pilot error. Brownout is a dangerous phenomenon that occurs when helicopters perform take-offs, approaches, and landings in dusty environments. Sand or dust particles get swept up in the rotor downwind and obscure the pilot’s vision of the terrain.

At issue with the applied problem of helicopter brownout was the lack of fundamental understanding of how the visual system copes with obscured scene viewing and object recognition. A surrogate situation in nature is camouflage, where animals have largely adapted three types of cues to hide themselves in plain sight: crypsis, disruptive patterning, and countershading. In nature and in operational environments, camouflaging an object of interest, or breaking its camouflage (i.e., being recognized despite camouflage), is important for survival. Camouflage has been studied at the behavioral level for more than a century. A rigorous, quantitative understanding of the relevant neural mechanisms and how they relate to the recognition of a camouflaged object was lacking.

**ACTION**

Former Neurophysiology Program Manager, Dr. Elmar Schmeisser, met with scientists and engineers from the U.S. Army Aeromedical Research Laboratory to discuss this applied challenge. The outcome was a plan to understand how visually confounded scenes affect the brain and whether interventions could improve object recognition under visually degraded conditions.

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This success was made possible by:

Dr. Frederick D. Gregory, Life Sciences Branch

Drs. Elmar Schmeisser and Liyi Dai, former Life Sciences Branch

Citations:

Starting in 2011, Professor Jay Hegdé from the Medical College of Georgia (now known as Augusta University) was initially funded by ARO to create an experimental paradigm to accurately and efficiently measure human psychophysical performance during camouflage-breaking. First, the research team utilized new computer graphical techniques developed for lighting, texture mapping, and synthesizing photorealistic images to incorporate all three types of natural camouflage cues. By allowing subjects to view, and learn, the background over multiple days, they were able to demonstrate that naive, nonprofessional subjects can be trained to accurately report whether a given camouflage scene contains a target (Figure 1). But it remained unclear whether experts actually detect the target or just vaguely sense that a scene is somehow different, without being able to find the target, per say.

After taking over the Neurophysiology Program, Dr. Gregory sought to bolster the search for the neurophysiological mechanisms underlying visual search performance by seeking out multidisciplinary opportunities from computer vision advances. As a result, he partnered with former ARO Program Manager, Dr. Liyi Dai, to support the Visual Search: A Comprehensive Treatment of Search conference in 2014, which was focused on the intersection between human visual search and computer vision. Professor Hegdé was one of the invited speakers and discussed his final results showing preliminary findings from functional magnetic resonance imaging suggesting that a particular pattern of brain network activity distinguishes camouflage-breaking from other visual search elements. As a result of workshop discussion and engagement, Dr. Gregory supported Professor Hegdé’s follow-on study beginning in 2015 to explore brain changes as subjects learned camouflage-breaking expertise and behavioral heuristics used during accurate detection. Professor Hegdé has expanded these approaches to include studies of visual pattern recognition using radiological images that may or may not contain cancer. He demonstrated in 2020 that nonprofessional subjects can be trained in his “deep learning” techniques and reliably perform aspects of medical image perception usually performed by highly trained medical experts.

**Figure 1:** (a) Process used to create camouflaged scenes with face targets. To create the stimuli, photographs of different types of natural backgrounds (e.g., a bed of mushrooms or foliage) were used as inputs to a texture synthesizer to create new instances of those background types. Each face target was textured using the same background type that it would be displayed against, but with a different instance of that type. Face targets were created with different rotations so they could be shown in any orientation from left profile through right profile. Face and background were then combined to create a camouflaged scene. (b, c) The graphs show discriminability, d', for stimuli with learned and novel backgrounds averaged across subjects in the pre- and post-training blocks for face (panel b) and digital embryo (panel c) targets. Error bars indicate ±1 standard error of the mean (SEM).

**RESULT**

This year, additional results were published from adult volunteers who were trained to break camouflage using Professor Hegdé’s deep-learning method. They received no specific training about how to pinpoint the target. Participants looked at digitally synthesized camouflage scenes with a 50-50 chance of containing a camouflaged target, like a human head or a novel 3D digital image (Figure 2). The relatively rapid method for training civilian novices also enabled camouflage-breakers to sense that something was amiss even when there was no specific target to identify. Professor Hegdé conducted a separate set of studies showing that this intuitive sense—that something is not quite right—is exhibited by experienced radiologists finding subtle changes in mammograms, sometimes years before there is a detectable lesion.

When the participants could look at the image for as long as they wanted, the reported location of the actual target was essentially indistinguishable from the actual target. Accuracy did not drop much when the viewing time was just 50 ms, which gives little time for even moving one’s eyes around. Even without specific training, subjects could do both equally well.

**WAY AHEAD**

Localization expertise evidently develops as a matter of course of acquiring target detection expertise using the deep-learning paradigm. Open questions remain about reliably training precise localization ability and the transfer of knowledge to other tasks. The potential ability to quickly instill object recognition abilities (within 50 ms) of Army-relevant scenes on demand is highly desirable. The next steps of this research include additional tests in human subjects as well as training artificial intelligence systems.

**Results**

- Determined that when subjects break camouflage, they can also localize the camouflaged target accurately, even though they had received no specific training in localizing the target.
- Proved that localization was significantly accurate when subjects viewed scenes as briefly as 50 ms, but more so when the subjects were able to freely view the scenes.

**Anticipated Impact**

Training camouflage-breaking expertise through deep learning may provide an operational advantage for visual-intensive tasks requiring object recognition under obscure conditions, such as the challenges imposed by piloting under brownout conditions.
This success was made possible by:

Dr. Frederick Gregory,
Life Sciences Branch

Dr. Liyi Dai, former Life Sciences Branch

Citations:


neural network algorithms to do similar tasks, which will facilitate transitioning to DEVCOM ARL for studies of subjects before, during, and after the training alongside intelligent agent teammates in hybrid teaming and dynamic search tasks.

SUCCESS STORY

Brain–Computer Interface for Enhancing Group Decision-Making

A new class of brain–computer interfaces (BCIs) has significantly increased the speed and the accuracy of group perceptual decision-making.

CHALLENGE

Making decisions—either individually or in groups—is an important aspect of everyday life. The degree to which one is confident that one’s decision is accurate (in the sense that it is a reflection of the probability of being correct) is known as metacognitive accuracy. Metacognitive processes allow decision-makers to be consciously or unconsciously aware of the likelihood of being correct, through the feeling called confidence. In difficult decision tasks where individuals tend to make poor decisions, groups usually perform better (e.g., wisdom of crowds). However, there are circumstances in which group decision-making can be suboptimal or even disadvantageous. One way to enhance group performance is to take into account the decision confidence that accompanies each individual opinion. However, there are many situations where rapid decisions are required, and waiting for each user to express their confidence after their decisions is not feasible. BCIs offer a potential solution.

Because brain signals differ widely from person to person, normally collaborative BCIs (cBCIs) do not integrate brain activity of multiple users. Instead, they typically give each user a classifier trained to best recognize decisions for that user. Group decisions are then formed by adding up the analogue outputs (the decision function value) of each classifier, so that outputs further away from the decision boundary have higher influence on the outcome. The error correction benefits of the wisdom of crowds were reduced by the imperfect interpretation of the user intentions associated with even the best BCIs. Therefore, for BCIs to become a deployable technology platform for team military operations, many fundamental barriers must be addressed.

ACTION

In 2018, the OUSD(R&E) Basic Research Office Director called on Tri-Service scientists to develop a research challenge on the topic of collaborative human–artificial intelligence (AI) decision-making in partnership with the UK Ministry of Defence. This research challenge would come to be known as the Bilateral Academic Research Initiative (BARI) pilot. This new international collaborative partnership would follow upon the successful launch of several bilateral partnerships between the U.S. and UK on Multidisciplinary University Research Initiative (MURI) projects. Dr. Gregory was one of the Army scientists tasked with contributing to development of the multidisciplinary basic research challenge, which provided an opportunity for both nations to drive foundational science of relevance to future missions involving human–AI teams.

At the same time, Dr. Gregory had already partnered with former ARO Program Manager, Dr. Dai, to lead one of the U.S.-UK MURI topics that was focused on basic research to drive future BCI capabilities.
With a programmatic emphasis on the underlying neural mechanisms involved in closed-loop neural interfaces, Dr. Gregory made sure that a stringent neuroscience emphasis was included in the ultimate topic call. U.S.-UK academic teams responded to the topic and the team, led by Professor Riccardo Poli from University of Essex and Professor Maryam Shanechi from University of Southern California, was awarded as the very first, and currently only, BARI-funded researchers. Dr. Gregory serves as the Tri-Service lead for management of the BARI effort in partnership with Ministry of Defence counterparts from the UK Defence Science & Technology Laboratory.

RESULT

A quantum leap in performance was obtained with a particular form of BCI developed by Professor Poli, which they call hybrid cBCIs because they use a combination of neural, behavioral, and physiological measurements. Here the objective was not to infer user intentions (these were reported by key presses), but to estimate the objective confidence (i.e., the true probability of being correct) of the members of a decision-making group on a decision-by-decision basis. This confidence was then used as a weight for the decision of the corresponding team member when aggregating individual contributions to form group decisions.

Over the years, early versions of this cBCI architecture were tested on a variety of tasks of increasing realism, including visual matching tasks, visual search with simple shapes, visual search with realistic stimuli, face recognition, and threat detection with video stimuli. In all cases, decisions supported by the cBCIs were superior (both in terms of accuracy and speed) in comparison to their non-BCI counterparts (standard majority or weighing decisions using self-reported confidence) when comparing equally sized groups.

Professor Poli’s implementation of cBCIs combine behavioral, physiological, and neural data. For the current accomplishment, his group examined electroencephalography signals associated with correct and incorrect decisions from all participants, as illustrated in Figure 4.

The team also determined the mean accuracies for individuals and groups of sizes 2 to 10. The different cBCI-based decision support systems were compared. Pairwise comparisons of the accuracies of all confidence estimation methods demonstrated that the cBCI-based, group-decision-making system with neural features, reaction time, and reported confidence is superior in performance to the other alternatives. The strategy gathers all information (neural signals, decisions, and reported confidence) available from any number of group members at any given time after the fastest responder has provided a decision. It then feeds such information to the appropriate types of decision support system.

**Figure 4:** The plots on the top are grand averages of the response-locked event-related potentials at the FCz channel location for correct (in blue) and incorrect (in red) decisions. Regions shaded in green show a significant difference (p < 0.05; Wilcoxon two-tailed signed rank test) between the correct and incorrect event-related potentials. The topographical scalp maps at the bottom represent the grand averages for correct and incorrect decisions and corresponding p-values obtained from the Wilcoxon two-tailed signed ranked test over all electrode locations at 300 and 80 ms before the response.

WAY AHEAD

For ethical reasons, many decisions in the military that can lead to possible fatalities cannot be made by an autonomous AI system. Humans must always stay in-the-loop. For this reason, it makes sense to augment and assist human decision-making using AI-based technologies. Only a fraction of real-world decision scenarios are time pressured, occur where there are only two options, and/or the perceptual information is available only for a short time. Instead, many Army decisions involve strategic decisions where resources (rather than time) are limited and more than two choices are available. Future effort will focus on extending cBCI to more complex problems in which, for example, decisions do not necessarily have a correct or incorrect choice, and can be based on perceptual information gained and decisions made in past trials. If successful, this work will facilitate translation to DEVCOM ARL for implementation in Soldier–system adaptation scenarios where collaborative decision-making is required.

**ARL Competencies:**

- Humans in Complex Systems

**Results**

- Determined that decision confidence can be measured from combined physiological, neural, and behavioral measures, providing the potential for an intelligent agent teammate to accurately assess human decision and decision-making capability in complex operations.

- Discovered that brain activity shows different patterns for correct and incorrect decisions, providing evidence for future Army-relevant studies of methods to improve object recognition performance.

- Established that groups assisted by cBCI make more accurate decisions than traditional groups.

**Anticipated Impact**

Future hybrid teams of humans and intelligent agents will be augmented by cBCIs in integrated and dynamic decision tasks in both training and operational environments.
Dr. Baker completed his undergraduate studies at Wright State University, receiving his B.S. in Physics in 2002. He trained as an atomic physicist at Tufts University, receiving his Ph.D. in Physics in 2009.

He came to ARO in 2010 as the Program Manager of the Atomic and Molecular Physics (AMP) Program.

SUCCESS STORY
Probing Topological Spin Liquids on a Programmable Quantum Simulator

Army-funded research demonstrated the first direct experimental observation of a topological quantum matter. Specifically, this breakthrough directly measured a quantum spin liquid (QSL) using two global measurements. More importantly, this experimental effort provides a new platform for investigating new forms of quantum matter and may lead to the development of topologically protected quantum information processing.

CHALLENGE
Researchers have long sought to demonstrate topological quantum matter or a quantum system with long-range entanglement. Topological systems have unique and interesting properties that can be exploited for future U.S. Army materials and systems. For instance, a major concern for quantum computing and quantum sensing is decoherence. Coherence is a sensitive relationship between the components of a quantum system, which are often the source of quantum advantage. A major research goal is therefore finding ways to reduce decoherence. Topological protection may provide a manner to protect coherence. Topological systems having long-range interactions, also referred to as global properties, which may provide protection against local environmental noise. Specifically, a local source of decoherence, such as heating, would have to affect the whole system simultaneously. In addition, global sources of noise often do not affect the coherence between the individual quantum parts. For these reasons, the realization and exploration of topological quantum matter is of great interest. As we can see from the discussed research here, the direct measurement of topological order, specifically a QSL, is challenging because the same effect that makes topological properties desirable, non-locality, makes those properties difficult to measure. This research result details how a probe for topological order can be used in a quantum system.

ACTION
In 2015, Dr. Baker engaged 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 (SI) 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 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 SI project was solicited and awarded in 2019 titled “Efficient light-matter interfaces for Rydberg arrays and entanglement in topological quantum networks.” During these two projects, significant technical challenges were overcome and significant demonstrations made. These demonstrations resulted in the DARPA Defense Sciences Office (DSO) establishing a new program titled “Optimization with noisy intermediate-scale quantum devices (ONISQ),” selecting the Vuletic/Lukin team as a centerpiece for this new project, and selecting ARO’s Drs. Baker and Gamble to participate in the execution of this new program. The goals of this DARPA program will be to demonstrate computational gains beyond what is possible classically with a focus on DoD-relevant problems. This new breakthrough in the direct observation of a QSL is the result of these prior ARO investments related to answering the Priority Research Question (PSQ) related to the realization of a quantum simulator for topological states.

Furthermore, the AMP Program Manager had sponsored a 2013 workshop on anyons and the potential for realizing topological particles in a quantum simulator. This internationally attended workshop helped develop a roadmap. Partnering with Dr. Marc Ulrich, a second workshop was held in 2015 that brought in a smaller group of condensed matter experts to discuss the potential for realizing topological particles in a solid-state system. Finally, this ARO investment led to the first topological Multidisciplinary University Research Initiative (MURI) that brought together leading experts in condensed matter and atomic physics.

![Fluorescence image of 219 atoms arranged on the links of a kagome lattice.](image)

**Figure 1:** (A) Fluorescence image of 219 atoms arranged on the links of a kagome lattice. The atoms, initially in the ground state |g⟩, evolve according to the many-body dynamics \( U(t) \). The final state of the atoms is determined via fluorescence imaging of ground-state atoms. Rydberg atoms are marked with red dimers on the bonds of the kagome lattice. (B) The blockade radius is adjusted to \( \text{Rb}/a = 2.4 \), by choosing \( \Omega = 2\pi \times 1.4 \) MHz and \( a = 3.9 \) µm such that all six nearest neighbors of an atom in |g⟩ are within the blockade radius Rb. A state consistent with the Rydberg blockade at maximal filling can then be viewed as a dimer covering of the kagome lattice, where each vertex is touched by exactly one dimer. (C) The QSL state corresponds to a coherent superposition of exponentially many dimer coverings. (D) Detuning \( \Delta(t) \) and Rabi frequency \( \Omega(t) \) used for quasi-adiabatic state preparation. (E) (Top) Average density of Rydberg excitations |n⟩ in the bulk of the system, excluding the outer three layers. (Bottom) Probabilities of empty vertices in the bulk (monomers), vertices attached to a single dimer or double dimers (weakly violating blockade). After \( \Delta/D \approx 3 \), the system reaches -1/4 filling, where most vertices are attached to a single dimer, consistent with an approximate dimer phase.

**RESULT**

A major reason quantum topological matter is of great interest is that often the particles involved are spread through the systems as an excitation. Though the system comprises atoms (individual local particles trapped in optical traps), they interact with each other at distances that form composite or global modes that provide protection from local environmental noise. This protection provides resistance to decoherence; however, it comes at a cost. The quantum information contained in the global mode is difficult to measure. The MURI team developed a method for measuring a topological system (e.g., a QSL), and demonstrated the first measurement of topological quantum matter.

This experiment setup uses laser light and a spatial light modulator to create a uniform 2D array of optical traps in a vacuum chamber. Roughly 200 alkali atoms are loaded from a cooled atomic gas into the array. The atoms are detected with automated software and reconfigured spatially to achieve full filling of the array and the array can be reconfigured into a variety of lattice geometries. A major feature of the experiment is creation of a Rydberg state. This is simply a laser excitation that is close to ionization, but is limited to an excited state around \( n = 100 \). Atoms that are adjacent are entangled through a process called a Rydberg blockade.

The key result of this effort was determining a method for measuring the QSL. To measure the QSL, two topological string operators are defined and measurements are made. There is a correspondence between the Rydberg atoms placed on the links of a kagome lattice, as shown in Figure 1A, and the dimer models on the kagome lattice. The Rydberg excitations can be viewed as “dimer bonds” that connect two adjacent vertices of the lattice (Figure 1B). Due to the Rydberg blockade, strong and properly tuned interactions constrain the density of excitations such that each vertex is touched by a maximum of one dimer. A QSL can emerge within this dimer–monomer model close to 1/4 filling and can be viewed as a coherent superposition of exponentially many degenerate dimer coverings with a small admixture of monomers (Figure 1C).

As mentioned, a defining property of a phase with topological order is that it cannot be probed locally. Therefore, to measure the QSL state, it is essential to measure topological string operators. The first

**Results**

- Demonstrated the first unambiguous experimental measurement of a QSL.
- Provided a breakthrough experimental test bed for exploring topological quantum matter.
- May demonstrate the first experimental topological qubit.
- Opened up an entirely new scientific research area suitable for novel topological materials, quantum computing, error correction, and quantum metrology.

**Anticipated Impact**

A major priority for the AMP Program is to realize fieldable quantum sensors, with a focus on sensors that provide navigation and timing. A major obstacle to this goal is isolating quantum sensors from environmental noise. Exploration of topological quantum matter could provide insight into material design with novel Army-relevant properties.
operator characterizes the effective dimer description and the second probes the quantum coherence between dimer states.

The study of closed string operators demonstrates an approximate dimer phase with quantum coherence between dimer coverings. While closed loops are indicative of topological order, it is important to compare their properties to those of open strings to distinguish topological effects from trivial ordering—the former being sensitive to the topology of the loop. This comparison is shown in Figure 2A and B, indicating several distinct regimes.

Open strings distinguish the target QSL phase from proximal phases. Therefore, the QSL can be identified as the unique phase where both order parameters vanish for long strings. It is not possible to classically simulate the quantum dynamics for the full experimental system, which limits comparing these results with theoretical approaches.

WAY AHEAD

The AMP Program identified a potential method for protecting quantum states from environmental noise using topological states. This foundational research provides a novel way for quantum computing to potentially provide new materials with designer properties. This result establishes a new test bed for the unambiguous experimental study of topological excitations. This research effort also explored potential encoding for topological qubits, which would represent an important achievement for reducing decoherence in quantum computing and quantum metrology. The researchers will continue to explore topological systems and increase precision and system size.

SUCCESS STORY

Quantum Approximate Bayesian Computation for Nuclear Magnetic Resonance Model Inference

Army-funded research led to the discovery of a hybrid algorithm that exploits near-term quantum computers to improve the nuclear magnetic resonance (NMR) spectroscopy used to identify small biological samples. This effort provides a powerful new diagnostic tool for identifying biomarkers of specific diseases and disorders.

CHALLENGE

NMR spectroscopy is a powerful technique, but has limitations in distinguishing uncatalogued particles. To address this computational challenge, a new hybrid classical–quantum algorithm was developed that resulted in a significant increase in accuracy and speed up. The researcher sought to exploit recent technological advances in the development of small-scale quantum computers that are capable of solving problems that cannot be tackled with classical computers. Currently, there are a limited number of algorithms that have been proposed for real-world problems. Analysis of many-body quantum systems is particularly challenging for classical computers due to the exponential scaling with the number of particles. Solving the problems relevant to chemistry and condensed matter physics is expected to be the first successful application of quantum computers.

ACTION

The AMP Program has been trying to exploit near-term noisy quantum (NISQ) computers, specifically looking to find areas were quantum approaches and classical machine learning (ML) could be combined. The AMP Program has made several joint investments with the Quantum Information Science (QIS) Program Manager (PM) to include quantum reservoir computing (QRC), quantum machine learning (QML), and quantum electrodynamic (QED) Hopfield neural networks. Furthermore, both the AMP and QIS PMs manage programs for DARPA DSO’s ONISQ program. Note that AMP investments in Rydberg lattices in the previous Success Story provided the experimental platform for this DARPA program. This awareness of near-term possibilities for quantum computers provided the background for the discussion of this project with Professor Eugene Demler of Harvard University. Professor Demler became aware of the U.S.
Army interest in demonstrable applications of quantum computing and through several discussions of a proposal for an NMR algorithm. Once support for this effort was provided, the result presented here followed within six months, demonstrating how ripe the area was for discovery. More cross-discipline efforts like this are being pursued to maximize the potential for discovery.

RESULT

Identifying molecular structure in biological and chemical samples is important for providing real-time situational awareness to the Soldier. NMR spectroscopy is a technique that is sensitive to local magnetic fields around atomic nuclei. Typically, samples are placed in a high magnetic field while driving RF transitions between the nuclear magnetic states of the system. Because these transitions are affected by the intramolecular magnetic fields around the atom and the interaction between the different nuclear spins, one can infer details about the electronic, and thus chemical, structure of a molecule. One of the main advantages of NMR is that it is nondestructive (in contrast to X-ray crystallography or mass spectrometry, for example). This makes NMR one of the most powerful analytical techniques available to biology, as it is suited for in vivo and in vitro studies. NMR can, for example, be used for identifying and quantifying small molecules in biological samples (serum, cerebral fluid, etc.). On the other hand, NMR experiments have limited spectral resolution. As such, there is a challenge in interpreting the data, because the extracted information is quite convoluted. Though the magnetic spectrum of a biological sample is observed, the goal of this effort is to learn the underlying microscopic Hamiltonian, and ultimately identify and quantify the chemical compounds. Although this inference is tractable for small molecules, it quickly becomes problematic, making inference a slow and error-prone procedure. The analysis can be simplified by incorporating an a priori spectral information in the parametric model. For that purpose, considerable attention has been devoted to determining NMR model parameters for relevant metabolites such as those found in plasma, cerebrospinal fluid, and mammalian brains.

The key insight of the researchers was the recognition of another class of problems from the quantum realm that can be solved efficiently on quantum computers: model inference for NMR spectroscopy, which is important for biological and medical research. These results are based on three interconnected studies. First, methods from classical ML were used to analyze a dataset of NMR spectra of small molecules. Specifically, ML was used to identify clusters of spectra and demonstrate that these clusters are correlated with the covalent structure of the molecules. Second, a simple and efficient method, aided by a quantum simulator, was used to extract the NMR spectrum of any hypothetical molecule described by a parametric Heisenberg model. Third, a simple variational Bayesian inference procedure was developed for estimating the Hamiltonian parameters of experimentally relevant NMR spectra.

WAY AHEAD

This result demonstrates a pragmatic application of near-term quantum simulation and how it can be used to provide better molecular identification using ML and NMR. This method may be extended to other types of experiments. NMR is hardly the only problem where one performs inference on spectroscopic data. For example, one can imagine combining resonant inelastic X-ray scattering (RIXS) data from strongly correlated electron systems with Fermi–Hubbard simulators based on ultra-cold atoms. Currently, RIXS data are analyzed by performing numerical studies of small clusters on classical computers. With cold atoms in optical lattices, it may be possible to create larger systems and study nonequilibrium dynamics corresponding to RIXS spectroscopy. This result provides a new method for improving model inference of NMR with a relatively modest amount of quantum resources. Similar to generic generative models such as Boltzmann machines, for which a more-efficient quantum version has been constructed, this result constructed an application-specific model from which a quantum machine can sample more efficiently than a classical computer. Model parameters are determined through a variational Bayesian approach with an informative prior, constructed by applying t-distributed stochastic neighbor embedding to a dataset of small molecules.

Figure 3: Method overview. A product state is taken with a given total magnetization $m$, according to $Q_j$. The latter can be chosen to minimize the variance of the estimand. After this initial preparation, the state under the Hamiltonian $H(j)$ evolves and measures the project back onto the $z$-basis at time $t$. By applying a fast Fourier transform to the estimate $S(t | j)$, one obtains the spectrum, which can be used to infer the parameters of the Hamiltonian.

Anticipated Impact

Developing new quantum algorithms that run on near-term quantum devices will impact many areas of science. Research that relies on computationally demanding solutions may find that these new quantum algorithms provide substantial improvement in speed and accuracy. Several U.S. Army applications can be directly impacted by these discoveries, including computer design, chemistry, and computation.
**QUANTUM OPTICS PROGRAM**

**Program Manager**

Dr. James Joseph

Dr. Joseph completed his undergraduate and graduate studies at Duke University, receiving his B.S.E in Physics and Electrical Engineering in 2001 and his Ph.D. in Atomic Molecular and Optical Physics in 2010. He worked as a research scientist at North Carolina State University and Duke University, and as a contractor for the Army supporting the Physics Branch at ARO. Dr. Joseph started at ARO in 2020 and currently manages the Modern Optics Program.

**Current Scientific Objectives**

1. Understand how integrated photonics can be utilized for quantum technologies and operate at the single photon level that, if successful, would enable advanced computation and communication technologies in a robust package optimized for size, weight, and power.

2. Explore light–matter interactions with cavity quantum electrodynamics to produce hybrid photonic–electronic states that, if successful, could lead to solid-state systems with optically driven properties that could be utilized for ultra-low-energy electronics or alternate energy applications.

3. Discover fundamental properties of how light interacts with subwavelength or ordered photonic structures that, if successful, would expand our ability to tune the properties of light on demand for a variety of applications including advanced sensing, optical data processing, and higher-order quantum state manipulation.

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**SUCCESS STORY**

**Higher-Dimensional Supersymmetric Microlaser Arrays**

Army-funded research at the University of Pennsylvania and Duke University discovered a way to create highly compact arrays of microlasers that combine the stability and coherence of single-mode lasers with the power performance of multimode lasers. This research has the potential to profoundly impact the performance of the Army’s existing photonics technology by providing a more powerful and stable light source.

**CHALLENGE**

Photonics technology has the potential to increase the speed of communication while reducing energy costs by storing and transmitting information with light rather than electrical circuits. To realize this potential, it is necessary to achieve light sources (i.e., lasers) of sufficient intensity that are compact, stable, and coherent. Stability and coherence are important for preserving the information manipulated by a photonic device. This is a challenging list of requirements. Traditionally, one would have to choose between stable single-mode lasers with narrow linewidths and higher-power multimode lasers, which are noisier and have poor coherence. One possible approach is to implement closely packed arrays of single-mode microlasers, which conceivably could combine the best of both systems. However, fundamentally, the wave-like nature of light gives rise to inevitable couplings between microlasers within the array, spoiling their collective, single-mode functionality.

**ACTION**

In 2016, Dr. Richard Hammond (former ARO Program Manager) held a two-day workshop at ARO where new fundamental ideas, with potential Army applications, were discussed. Supersymmetric optics, then a new field, was pioneered by the team of Dr. Demetri Christodoulides at the University of Central Florida, Dr. Ramy El-Ganainy at Michigan Technological University, and Dr. Mercedeh Khajavikhan at the University of Southern California. With Army funding, Dr. Christodoulides and his team first experimentally demonstrated it was possible to utilize the concepts of supersymmetry in optics to design more-efficient laser arrays in one dimension.

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This success was made possible by:

Dr. James Joseph, Physics Branch
Dr. Richard Hammond, Physics Branch (Retired)

**Citations:**


Dr. Hammond continued to explore this area by engaging the broader academic community in a series of discussions. In 2018 and 2019, ARO awarded two efforts lead by Dr. Natalia Litchinitser at Duke University and Dr. Liang Feng at the University of Pennsylvania, respectively. These efforts produced a greater understanding of the fundamental concepts of gain and loss in coupled photonic systems and resulted in finer experimental control for fabricating laser arrays. These efforts constitute the subject of this Success Story.

RESULT

Dr. Feng from the University of Pennsylvania and Dr. Litchinitser of Duke University were able to control the mutual couplings of the microlasers in an array by borrowing an idea from particle physics known as supersymmetry (SUSY). By employing this key insight, they were able to successfully design and fabricate a 2D array of closely packed microlasers with the stability of a single microlaser. The 2D SUSY microlaser array has significant enhancements in relation to traditional microlaser arrays including a lower lasing threshold, lower beam divergence, and increased energy density.

SUSY was first introduced to unify all physical interactions in nature, including the strong, electromagnetic, weak, and gravitational forces, as well as solve the problem of the Higgs boson’s unexpectedly light mass. Under SUSY, each particle in the Standard Model is paired with a supersymmetric partner particle that differs in spin by a half integer. In this regime, each boson is paired with a fermion and vice versa. Outside particle physics, the mathematical framework of SUSY has found application in condensed matter, optics, and photonics. In this SUSY-inspired design, arrays of dissipative superpartner microlasers are coupled to the main 2D laser array. This arrangement forces the coupled microlasers to phase lock and coherently oscillate in a fundamental, in-phase mode. This in turn causes the array to behave collectively as a powerful, single-mode laser.

The main 2D array comprises five columns by five rows of identical microring lasers made of indium gallium arsenide phosphide (InGaAsP) quantum wells, resulting in 25 transverse modes with a closely spaced spectrum. Coupled to this are 3 × 5 and 2 × 3 arrays of identical elements with the same resonant frequency as the main array, as well as three individual auxiliary partner microrings. A pictorial representation of the system is shown in Figure 1. The spectrum of the superpartners is identical to that of the main array, apart from the fundamental in-phase mode. The superpartners are made dissipative by pumping them below the lasing threshold. Strategically controlling the coupling of the main array with its dissipative superpartners and auxiliary partner microrings, by matching both the spectral frequencies and mode distributions, suppresses all but the fundamental transverse mode, yielding efficient single-mode lasing with high radiance, a single frequency, and substantial power enhancement. In the fundamental in-phase mode, all 25 individual microlasers in the main array oscillate and contribute to a factor of 25 power enhancement over a single microlaser. This research builds on previous work by collaboration on 1D superpartner laser arrays.

The study also shows that the technique is compatible with the team’s earlier research on vortex lasers, which can precisely control orbital angular momentum (OAM). OAM quantizes the manner in which a laser beam spirals around its axis of travel, and is defined by both direction of spiral and order, or magnitude, of spin. The SUSY microlaser array allows for the required control of OAM by strategically designing the angular grating inscribed on each microring while improving the total power output. By matching the order of the angular grating with the order of the resonant mode, all 25 angular momentum associated with emission become zero. The desired phase variation and polarization distribution are collectively transferred to the laser beam emitted from the SUSY microlaser array, thus facilitating single-frequency, high-radiance vortex lasing with a factor of 20.2 power enhancement. Additionally, with the added degree of freedom offered by allowing angular momentum into the beam, the researchers can select the direction and order of the OAM mode, which represents additional information pathways that can be encoded within the optical signal. This could enable photonic systems encoded at higher densities than previously imagined.

Figure 1: A SUSY microlaser array. The array consists of a 5 × 5 main array of evanescently coupled microring lasers (red), coupled with its two dissipative superpartner arrays and three auxiliary partner microrings (blue). Adapted from Qiao et al. (2021).

Results

- Developed a method to create 2D laser arrays as a high-power, stable, coherent light source for photonics applications.
- Published in the journal Science and featured in news releases.
- Results conveyed to Army leadership reported in the Morning Report.
- Work featured in an ARO summer workshop on non-Hermitian optics.

Anticipated Impact

This work on coupled photonic systems has demonstrated new capabilities in laser arrays and promises advanced sensing capabilities for systems where thermal emissions need to be considered.
WAY AHEAD

The technology developed in this project is a generic approach applicable to higher-dimensional SUSY microlaser arrays. The collaboration from the University of Pennsylvania and Duke envisions extending this approach to larger arrays as well as arrays in three dimensions. There are also plans to further develop and refine the OAM structures for more-exquisite control and faster switching.

Further, in 2020, Dr. Joseph decided to explore the role of gain and loss in coupled resonators for sensing applications by awarding a 3-year grant to Dr. Gururaj Naik at the Rice University. This ongoing work will explore the limits of asymmetry with regard to the emission of thermal radiation. In part due to the success of these efforts, Dr. Feng was awarded a Defense University Research Instrumentation Program (DURIP) in the 2022 fiscal cycle. Finally, in the summer of 2021, Drs. Joseph and Naik ran a workshop on non-Hermitian optics. Drs. Christodoulides, Feng, Litchinitser, El-Ganainy, and Khajavikhan all participated and helped run the workshop, with Dr. Christodoulides providing the keynote address. This workshop will inform future funding decisions for the Army's Modern Optics Program.

SUCCESS STORY

Interactions of the Twisted Light with Quantum Systems

Army-funded research at The George Washington University developed a new fundamental understanding of optical vortices, which will lead to increasingly tunable and flexible technologies for producing light with a new degree of freedom, namely, OAM, or twisted light. Tunable twisted light has the potential to increase the bandwidth in optical communications, provide enhanced sensitivity and selectivity for optical sensors, and provide a means to control the release of energy in nuclear isotopes.

CHALLENGE

Vortices are common in nature, from circulation in rivers and oceans, to spiral galaxies, to quantized vortices in Bose–Einstein condensates (BECs). Over the past 30 years, the optics community has identified and advanced the concept of vortices in light. The mathematical equations describing optical vortices are similar to hydrodynamic equations, which reveal a flow singularity in a fluid vortex, except with light, the singularity is in the phase of the light and appears as an isolated dark spot or donut shape. To investigate how twisted light interacts with quantum systems such as atoms, molecules, ions, or atomic nuclei, researchers must provide exquisite control of the twisted light properties. Thus, to develop this exquisite control, we must advance our fundamental understanding of the nature of twisted light.

ACTION

In 2015 and 2016, Dr. Richard Hammond (former ARO Program Manager) sponsored two conferences on “Laser-driven radiation sources for nuclear applications” and “Isotope-based energy sources,” respectively. The conferences, held at the Foggy Bottom campus of The George Washington University and organized by Dr. Andrei Afanasev at The George Washington University, were attended by DEVCOM ARL personnel and leading academic experts. The objective is to fund a workshop to review the current status and identify new directions in the area of laser-driven sources of radiation energetic enough to become relevant to physics phenomena at nuclear scales. One promising direction to explore that emerged from these conferences was to examine the role OAM plays in nuclear processes like energy conversion from nuclear isotopes.

Then in 2017, Dr. Hammond initiated a 4-year Cooperative Agreement at the University of Nebraska to study the controlled release of energy of nuclear isomers. This effort studied how to optically control the storage and release of energy from nuclear isomers. Nuclear isotopes store considerably higher energy density per unit mass than chemicals, by a factor of about 100,000, and isotope-based batteries would not require replacement over the lifetimes of the radioactive sources, which may extend to hundreds or thousands of years.

Later in 2019, Dr. Hammond requested that Dr. Afanasev explore the role twisted light plays in light–matter interactions. This ongoing effort is the subject of this Success Story. Initial studies showed promise beyond energy storage applications. With the encouragement of ARO Program Mangers, Dr. Afanasev has also applied for and received additional funds to sponsor one high school student and one undergraduate student under the High School Apprenticeship Program/University Research Apprenticeship Program (HSAP/URAP).
RESULT

The main objective of this project is to develop a theoretical and computational framework for the interaction of twisted photons with quantum systems. Researchers from The George Washington University, with Army funding and in collaboration with the College of William & Mary, studied the effect of twisted photon absorption on cold-trapped 40Ca+ ions. It was found that the transverse impulse given to a target atom depends directly on the offset distance from the vortex line of the photon as well as the total angular momentum of the twisted photon. The density of the photon state decreases near the vortex line, but the local momentum relative to the probability density in the same region can be very large. A sufficiently small probe, like an ion, within this region has a low probability of interaction, but such an interaction will create a large transverse momentum impulse (Figure 2). In some circumstances, this transverse impulse will be considerably larger than the longitudinal momentum of the Fourier components of the twisted photon. Researchers named the momentum transfer in this case a superkick. The angular momentum that does not transfer into internal electronic excitations is passed to the target atom’s center-of-mass motion. For this study, researchers calculated the photoabsorption of twisted photons on 40Ca+ ions suspended in a segmented Paul electromagnetic trap.

In a follow-on study, researchers investigated the photodisintegration of a deuteron, which is the process whereby a 2H nucleus absorbs a photon (gamma ray) and dissociates into its constituent neutron and proton. The transverse recoil momentum for this reaction increases with smaller values of impact parameter. Here the momentum transfer can be classified as a superkick from the previous definition. The effect of the superkick is seen by analyzing the energy spectrum of the dissociated protons and neutrons. At energies near the reaction threshold, the neutron–proton pair is produced with a small relative momentum and moves almost parallel to the incident photon. Since the additional recoil momentum from twisted gamma rays is purely transverse, observing either of the two nucleons emerge with excess energy at large relative to the beam would indicate a superkick. Tight focusing of twisted gamma-ray beams is essential for such measurements.

In parallel with these experimental efforts, Dr. Afanasev developed a theoretical formalism to describe the atomic response from twisted photon excitations. The optical beam has contributions from longitudinal (along a beam’s propagation direction) and transverse electromagnetic fields. Electric dipole transitions only occur for atomic transitions with no change in their magnetic quantum number, but higher-order multipoles do have contributions for transition between magnetic quantum numbers. A spin density matrix can be constructed describing the allowed and forbidden transitions corresponding to large OAM transfers, or superkicks. From this work, Dr. Afanasev and his collaborators discovered that the transitions are sensitive to the angular momentum of the incident optical field. The formalism provides a means to pair the appropriate tunable field parameters expanded to include OAM with localized atomic probes like trapped and cooled ions.

WAY AHEAD

The collaboration plans to further study the observable superkick phenomenon by using final-state rather than initial-state localization. They foresee the theoretical tools developed in this work being extended beyond energy storage in nuclear isomers and into the realm of integrated photonics-based information processing (such as neural network-based accelerators and photonic tensor cores), adaptive sensing, analog optical and photonic processors, adaptive optics, artificial intelligence through holography, optical encryption, and free-space communication. It is also the intention of Dr. Joseph to sponsor and engage with future workshops and conference on twisted light–matter interaction to inform funding decisions within the Modern Optics Program.
SUCCESS STORY
Bringing Quantum Advantages Closer to Reality: A Mathematical Approach

Army researchers developed theoretical approaches for accelerating our ability to execute hybrid quantum-classical algorithms on small quantum computers and elucidating how to best map the operations prescribed by quantum algorithms to small quantum computers, which lack all-to-all connectivity of the constituent quantum information processing units, called qubits. As qubit-based quantum hardware development continues to improve, theoretical advances such as these will be integral to the Army’s ability to exploit quantum processors as early as possible for the realization of beyond classical capabilities in computing, sensing, and communication.

CHALLENGE

While we have small-scale quantum information processing experiments functioning in labs today, we will need to achieve significant hardware advances for these experiments to evolve into devices capable of executing the sophisticated quantum operations we need for Army- and DoD-relevant applications. While we are investing in relevant quantum hardware experimental development, that alone is not the only pathway to bring us closer to realizing quantum-based beyond classical capabilities as quickly as possible. Developing better theoretical understandings of how to formulate quantum algorithms that can produce useful results even with small numbers of quantum operations and how to best execute those operations on a small quantum processor are open challenges.

ACTION

A primary long-term goal of the quantum information science community is to build large-scale quantum systems such as quantum computers and distributed quantum networks, which can carry out operations sophisticated enough to enable revolutionary capabilities not possible with classical systems. Often, this goal is thought of as running in parallel with efforts to develop new quantum algorithms, which will ultimately run on these systems. While experimental physicists, engineers,
and materials scientists work to advance quantum hardware, quantum algorithm developers from the physics, mathematics, and computer science communities work to derive new quantum algorithms to expand the application spaces for which quantum systems can potentially provide advantages. While these lines of work do not often have to be conducted in close collaboration, ultimately these communities do need each other—without quantum algorithms detailing how to use the quantum properties of matter to enable beyond classical capabilities, we would not need quantum hardware like computers and networks; yet, without the quantum hardware to implement them, quantum algorithms are essentially useless.

As experimental work has progressed over the last several decades, however, it has become increasingly clear that building these large quantum systems is incredibly challenging and realizing them is likely still decades away. In response to this, questions naturally began to emerge related to potential use cases for near-term non-error-corrected quantum computers. In 2017, Dr. Gamble began pursuing questions related to the broader development of quantum algorithms and their relation to these noisy intermediate-scale quantum (NISQ) devices. In particular, Dr. Gamble began to explore projects aiming to elucidate how quantum algorithms, independent of target application, may be designed to provide advantages with the lowest possible overhead related to the quantum processes as possible. In other words, since it is becoming increasingly clear we will be in the realm of NISQ devices for the foreseeable future, how can we best design and implement algorithms with hardware limitations in mind? How can we better bring hardware limitation considerations to the quantum algorithm community to both maximize productivity in the near term and position ourselves to best execute algorithms on error-corrected quantum hardware when it becomes available?

Dr. Gamble sought and ultimately acquired a plus up to the Quantum Information Science Program to pursue this and other related lines of inquiry in quantum algorithms. As a result, she was able to fund a large, multi-principal investigator (PI) initiative led by Professor Aram Harrow from the Massachusetts Institute of Technology. The theory team commenced their work on the multiyear project in late 2017.

**RESULT**

Since commencing their work, the quantum algorithm team has made strides in a variety of areas related to quantum algorithm development. In FY21, the team was able to make significant advances in two areas: (1) theoretically showing that utilizing a particular approach to hybrid quantum classical optimization problems has merit and (2) developing theory to guide how to execute quantum algorithms on devices with limited physical connectivity in quantum hardware processors.

Result 1: “Variational algorithms,” which have both classical and quantum components working hand-in-hand in hybrid configurations, were developed with the philosophy that even algorithms with a minimal number of quantum steps could be useful and provide performance beyond what is accessible with 100% classical algorithms. Types of variational algorithms have been proposed for quantum simulation, combinatorial optimization, and machine learning applications. Within these algorithms, however, it is not always apparent what strategy is best and, in particular, if sometimes undertaking slightly more complicated steps in parts of the algorithm is actually helpful for overall performance. Professor Harrow’s team successfully answered this question for the case of mathematical analytic gradient measurements, where a long-standing question had been whether taking the time to calculate these gradients is ever beneficial in the overall algorithmic process. Not only was the team able to answer this question in the affirmative, showing that performing stochastic gradient descent provably converges to an optimum answer faster than any algorithm that only measures other quantities, but they also derived the upper bounds on the cost of doing these calculations when the algorithm is essentially close to an answer. These results are crucial for guiding expectations on the performance of these algorithms for Army-relevant problems, especially those related to logistics and optimization.

Result 2: Qubits are the fundamental unit of quantum information processing and analogous to bits in classical computing. While future, fault-tolerant, error-corrected quantum computers will

**Results**

- Made theoretical advances that will facilitate the execution of quantum algorithms on near-term, error-prone quantum hardware. Since large-scale, fault-tolerant, error-corrected quantum hardware is likely still decades away, these advances will likely accelerate the timetable on which the Army can leverage quantum-based advances for improved information processing on and off the battlefield, especially in areas related to logistics and optimization.

- Showed that, for a certain circumstance, adding additional steps into hybrid quantum–classical calculations improves the overall performance of the computation, despite the added complexity.

- Developed guidelines for mapping the steps of quantum calculations to physically imperfect quantum hardware, specifically hardware in which all of the qubits, the fundamental unit of information processing in quantum systems, do not have all-to-all connectivity.

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**Figure 1:** Example quantum circuit from Result 2. Here, each horizontal line represents a qubit and the black vertical lines connecting certain qubits represent quantum operations, or “gates.” The red vertical lines separate where one layer ends and the next ones begins in the team’s approach to mapping the implementation of quantum algorithms to quantum systems where not all qubits are connected one another. Adapted from Lin et al. (2021).
likely have qubits that are all connected to one another in some fashion, large processors with full all-to-all qubit connectivity are likely still decades away. This year, Professor Harrow’s team successfully developed a heuristic approach for mapping the qubit operations prescribed by an algorithm to the physical qubits of connectivity-limited devices, thereby giving experimentalists a tool to guide use when executing small quantum algorithms on near-term, imperfect hardware (Figure 1). In particular, their approach uses a type of graph theory and, when compared to two other recent, high-performing algorithms, they found that their spectral graph theory approach resulted in implementations that used fewer quantum operations while still having scalable space and runtime characteristics. This result is poised to aid in the adaptation of quantum algorithms for Army-relevant problems to be run on NISQ hardware, potentially enabling these algorithms to produce results in the nearer term than they would without this heuristic approach.

**WAY AHEAD**

Dr. Harrow’s team will continue to develop algorithms and approaches that bridge the gap between near-term, imperfect hardware and fully fault-tolerant, error-corrected quantum systems. As the Army moves to adapt quantum algorithms for Army-relevant problems at DEVCOM ARL and the DEVCOM Centers over the course of the next several years, integrating approaches such as Professor Harrow’s will likely be crucial for success.

**SUCCESS STORY**

**Developing a Quantum Information Science Workforce, One Student at a Time**

The current rate of expansion of research- and industry-based efforts in quantum information science is outpacing the rate at which the United States can train and disseminate a properly educated workforce. Through the Army’s Educational and Outreach Program (AEOP), ARO is able to support apprenticeships for high school and undergraduate students, and the Quantum Information Science Program routinely takes advantage of this support. Beginning in 2019, one researcher used these Army student funds as leverage with industry and philanthropic partners to enable the funding of a full Summer Quantum Camp, educating classes of students. The Army’s modest investments catalyzed the program’s enormous success, which has attracted the attention of the White House’s Office of Science and Technology Policy (OSTP), leading to further opportunities for the Army to influence quantum information science policy at a national level.

**CHALLENGE**

Educating a workforce in quantum information science has many unique difficulties compared to other fields. To start, initial quantum mechanics courses are typically limited to upper-level physics major curriculums, vastly limiting the exposure most students are able to receive to the foundational science of the field. Additionally, quantum information science, while built on the physics of quantum mechanics, is itself a highly interdisciplinary field encompassing facets of not only physics, but computer and information science, materials science, and engineering. Finally, the non-intuitive nature of quantum physics can act as a barrier for some students to pursue the field, even if they attend schools with quantum information science programs, which are typically limited to top-tier R1 institutions. The AEOP’s High School and Undergraduate Apprenticeship Program (HSAP/URAP) helps bring high school and undergraduate students into some of the leading quantum information science research groups and laboratories every summer, yet there are significantly more students who are poised to benefit from this program than the program can support.

**ACTION**

Each year, Dr. Gamble supports as many HSAP/URAP students as possible in an attempt to grow the quantum information science workforce and expose students to Army- and DoD-relevant research. Beginning in the summer of 2019, ARO quantum information science principal investigator Javad Shabani at New York University (NYU) leveraged his annual HSAP/URAP funds to actively engage with both industrial and philanthropic partners to successfully leverage $10,500 in HSAP/URAP funds to obtain more than an additional $50,000 in support for a full NYU Summer Quantum Camp. This support continued in 2020 and 2021. In 2019, Dr. Gamble and the AEOP Program Manager (PM) traveled to NYU at the end of the camp to hear the students’ final presentations, see the hardware demos some of them constructed as part of their projects, and talk with them about future opportunities and plans. While the 2020 and 2021 camps have been...
virtual due to COVID-19, Dr. Gamble and the AEOP PM, now Ms. Ivory Chaney, have remained engaged with the quantum campers through the annual presentation symposiums and ensure that each Summer Quantum Camp class is aware of the follow-on opportunities in quantum information science available through the Army.

RESULT

Over the three summers from 2019 to 2021, Professor Shabani’s Summer Quantum Camp has supported a total of 47 high school and undergraduate apprenticeships, with some students returning for multiple years to further build their skills (there have been 41 unique attendees). High school camp alumni have gone on to declare physics and engineering majors in college, and undergraduate camp alumni have declared double majors or switched majors to more quantum information science–relevant fields after their camp experiences. Four undergraduate participants have won IBM “Qiskit Hackathons,” a hacking competition based on IBM’s Qiskit quantum programming language, and former undergraduate alumni are now participating in some of the premier graduate programs in the country. Additionally, one alumna who participated in the program in 2019 and 2020 returned in 2021 to share her work, begun under the program, writing a textbook, Quantum computing for beginners. Since the close of the 2021 program, the student and Professor Shabani have signed a publication agreement to formally publish and distribute this textbook.

Quantum information science is not unique, yet is perhaps a leading example of a field that must diversify to develop and build a workforce that reflects the diversity and inclusivity of America to ultimately succeed to the best of our abilities. NYU’s program is making exemplary progress in this area with respect to the participation of women, an underrepresented group in the quantum sciences, with 18 of the 41 participants identifying as female.

In 2020, Dr. Gamble highlighted the success of NYU’s program at a meeting hosted by the White House OSTP. The magnitude of the impact of the program was significant enough such that Dr. Gamble’s expertise was sought after as a member of an OSTP working group focused on Workforce Development in Quantum Information Science and Engineering. Through her role in this group, she is ensuring the United States cultivates and maintains a diverse and inclusive talent pool for the quantum sciences capable of meeting future Army, DoD, government, and civilian needs.

WAY AHEAD

ARO and Professor Shabani plan to continue Army support of his HSAP/URAP and Summer Quantum Camp efforts. These programs engage future scientists at the individual student level. When combined with Army representation at the national level, such as with Dr. Gamble’s participation in the OSTP Workforce Development in Quantum Information Science and Engineering working group, the programs will position the Army to develop a highly educated and diverse workforce in the quantum sciences poised to tackle Army and DoD challenges well into the future.

Results

- Leveraged the HSAP/URAP PI’s program funds to secure support for Summer Quantum Camps from FY19–21, resulting in 47 summer positions for high school and undergraduate students to become familiar with and accelerate their educations in quantum information science.

- Led to Summer Quantum Camp alumni students now majoring in physics programs and going to graduate school in quantum information science related fields, and one alumna in the process of publishing a textbook, Quantum computing for beginners.

- Drew the attention of the White House OSTP and led to Dr. Gamble’s inclusion in an OSTP working group targeting Workforce Development in Quantum Information Science and Engineering.

Anticipated Impact

These efforts are directly contributing to building and strengthening a diverse and inclusive quantum-educated workforce poised to tackle Army- and DoD-relevant problems, a workforce that will be necessary to ensure the operationalization of quantum information science.
SOLID STATE PHYSICS PROGRAM

Program Manager
Dr. Marc Ulrich
Chief, Electronics Branch

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 what was then called Condensed Matter Physics (now Solid State Physics) and was promoted to the additional role of Chief, Physics Branch in 2008. He transferred from Chief, Physics Branch to Chief, Electronics Branch in 2020.

Current Scientific Objectives

1. Strongly couple light and solid-state matter to fundamentally alter the physics of solid-state systems that, if successful, will discover concepts profitable for sensing and information processing.

2. Determine how to induce dissipationless current at ambient conditions without relying on superconductivity that, if successful, will enable ultra-efficient electronic device concepts.

3. Develop methodologies for probing the physics governing the interaction between topological electronic states and magnetic states that, if successful, will enable novel electronic/spintronic device concepts to be conceived.

SUCCESS STORY
Jekyll and Hyde Electronic Devices

ARO-funded work at the Massachusetts Institute of Technology (MIT) has, in concert with funding from other agencies, resulted in a device that can transform from one type of device into another. By tuning the voltages on several contacts, the material properties and thus the electronic device functionality are completely altered. This success indicates that novel electronic materials can provide a route to a new form of reconfigurable electronics that may be of value for the future of the Army’s Intelligence and Mission Command functional concepts.

CHALLENGE

For years, even decades, there have been many novel electronic materials proposed and realized. However, the vast majority of these have failed to have a technological impact due in large part to the incompatibility between the disparate materials necessary to constitute a functional electronic device. For example, when a functional material such as a ferroelectric is contacted by a metal electrode, there can be poor contact, delamination, deleterious chemical reactions, incompatible processing requirements, interface-induced defects, and other details that prevent the functionality of the material from being effectively harnessed.

ACTION

This challenge of chemical and functional compatibility was brought into sharp focus in the Solid State Physics Program during a season in which the program was aggressively seeking to discover a material heterostructure where Majorana fermions were observable and controllable. Majorana fermions are an esoteric and elusive particle that had been shown mathematically to provide a strong opportunity for scalable quantum computing. To realize them in solid-state forms required a virtually perfect interface between a topological material and a superconductor. Dr. Ulrich’s initial strategy was to employ old-school surface science to a small promising set of topological and superconducting materials. By understanding the chemistry and physics of the interface at an atomistic level, both theoretically and experimentally, in the context of the fabrication strategies, one should be able to engineer an interface suitable for the observation, study, and manipulation of Majorana fermions.
During this endeavor, Dr. Ulrich was made aware of efforts on a fascinating 2D material, tungsten ditelluride (WTe$_2$). It had been shown that this material could be a superconductor or it could be a quantum spin Hall insulator (QSHI), a topological state, depending on an electric field to which it is subjected. This led Dr. Ulrich to ask, “What if the interface between a superconductor and a topological material were made from the same material?” Specifically, if one could choose for a single material to be a superconductor or a QSHI at will, then one could design a topological–superconductor interface for Majorana fermions without having an interface at all. While this presented other difficulties, it was a novel approach that could do an end run around the very challenging matters of material compatibility in heterostructures. As a result, Dr. Ulrich sought out and funded work at Harvard University and MIT.

Since that time, two other important discoveries have been made in graphene, a single-atom-thick form of carbon that has made many headlines since its discovery in 2004. The first was the discovery by Professor Pablo Jarillo-Herrero—the co-principal investigator on the ARO-funded WTe$_2$ project—that superconductivity can be induced in a twisted two-layer form of graphene. The second was that magnetism can also be induced in layered forms of graphene. Conventional knowledge was that carbon could not host either of these states of matter. It was now clear that, for some materials, characteristics are not fixed properties but can be very flexible. This led Dr. Ulrich to propose a Multidisciplinary University Research Initiative (MURI) with the objective of devising entire devices—and potentially even circuits—using a single material. He was not aware that independently, Professor Jarillo-Herrero had begun working on trying it in graphene.

![Figure 1](attachment:image.png)

**Figure 1.** (a) The Jekyll-and-Hyde device schematic, where the twisted bilayer graphene (“MATBG”) is contacted by six electrodes (yellow). Two gold pads on top with applied voltages, $V_{tg1}$ and $V_{tg2}$, form two regions in which the graphene is tuned with an electric field in concert with the back gate underneath. The region outside these two (also between them) can be a third region that is not tuned. (b) The phase diagram for MATBG as a function of electrical bias, where the x-axis refers to the filling of the various electronic “bands” that emerge from the twisting of bilayer graphene and are a proxy for the applied three voltages. Notice that the graphene can be metallic, insulating, or superconducting depending on the temperature and applied voltages. At sufficiently low temperatures, all phases are accessible simultaneously in a single device. Adapted from Rodan-Legrain et al. (2021).

**Results**

- Demonstrated that electronically agile materials can circumvent material incompatibility issues and enable new device concepts.
- Demonstrated that electronically agile materials allow devices to be reconfigured on the fly.

**Anticipated Impact**

Advances in this area may lead to electronics that reconfigure for multiple applications such as energy harvesting, sensing, and information processing. Furthermore, by making new materials available, it may provide a route to electronic technologies that have lower manufacturing and environmental costs than traditional semiconductor materials.
This success was made possible by:

Dr. Marc Ulrich, Electronics Branch
Dr. Pani Varanasi, Materials Science Branch

Citations:


energy levels, restricting the number of electrons that can reside on the “island,” as shown in Figure 2a. Figure 2b shows the Coulomb blockage characteristics typical of a single-electron transistor. This result demonstrates that electronic devices can be constructed from a single material and that such devices have reconfigurable functions.

WAY AHEAD

In summer 2021, a MURI was competitively awarded to Harvard to pursue device concepts from single materials such as those described previously. This team will harness superfluidity, topological properties, and plasmonic and hydrodynamic physics to devise device concepts for terahertz emission, topological superconducting devices, and entanglement. The MURI was awarded as a Cooperative Agreement to foster interactions and collaboration with DEVCOM ARL. Leaving the question of moral agency of electronic devices aside, we anticipate more electronic forms of Dr. Jekyll and Mr. Hyde that can display vastly different properties in the same material.

SUCCESS STORY

Coherent Optical Control of Material Properties

With funding from ARO, California Institute of Technology researchers have demonstrated significant control of the optical and electronic properties of an insulator without accompanying detrimental effects such as heating. Illuminating a layered insulator with laser light below all allowed optical transitions, the nonlinear optical properties and bandgap of the material are coherently changed. Since the change in optical properties closely follows the envelope of the illumination, it demonstrates a technique for coherent (and thus ultrafast) optical control of materials profitable for functional photonic integrated circuits.

CHALLENGE

Traditionally, material properties are fixed characteristics of a material—one takes what is available based on the chemistry of bonding between atoms and the physics of electrons, vibrations, etc., present within the material. These can be manipulated to a degree with electric and magnetic fields, strain, temperature, or other parameters. A highly desirable knob to add to controlling materials properties is light due to, among other things, the extreme speed with which it can be turned on and off. While some control of material properties via light has been achieved, the majority involve processes that do not coherently follow the illumination. For example, the dynamics of electrons, holes, and thermal excitations resulting from illumination are material properties independent of the light and typically orders of magnitude slower than the light’s switching speed.

ACTION

While optical manipulation of materials has been around for decades, as well as advances in materials—including synthetic platforms such as cold atomic gases, superconducting qubits, etc.—coherent quantum control of optical properties is more elusive. However, techniques and materials theory during the 2000s and beyond have allowed endeavors in what is referred to as Floquet engineering. Just as the electronic properties of a crystalline material result largely from the spatially periodic potential they experience, they should be equally affected by a temporal periodic potential. There are many time-periodic perturbations that can be applied to a material, but laser light is extraordinarily versatile and widely available across a great deal of the electromagnetic spectrum. To advance knowledge toward coherent control of solid-state materials in this manner, Program Managers Drs. Marc Ulrich

Figure 2: (a) Energy/position schematic showing the operation of a single-electron transistor. Insulating barriers between electrodes left and right create an island where electronic states are energetically isolated. Adjusting the voltage on the left and right electrodes causes the island to charge or discharge one electron at a time when energy levels align with that of each electrode. (b) The characteristic Coulomb diamonds showing charging and discharging of the island with single electrons: (left to right) each dark-blue diamond represents the addition of one electron to the island. Adapted from Rodan-Legrain et al. (2021).
and Pani Varanasi realized a MURI-sized effort was needed to seed this important field with a strong multidisciplinary team. They created a MURI topic seeking “hidden” properties of materials coherently driven by electromagnetic radiation. Professor David Hsieh of the California Institute of Technology and his team won the competition and efforts under the grant began in 2017.

**RESULT**

During the course of the studies, the team identified some insulating trichalcogenides as having a strong potential for the discovery of light-induced properties due to their bandgaps being large, being free of in-gap states, and having a charge transfer character, which allows strong mixing by light. The trichalcogenide manganese phosphorus trisulfide (MnPS₃) (Figure 3) has a 3.1-eV bandgap and undergoes magnetic ordering below a temperature of 78 K into an antiferromagnetic structure that breaks inversion symmetry. These properties make the material promising for demonstrating Floquet engineering of optical properties. The broken inversion symmetry allows properties to be probed by second-harmonic generation, the 3.1-eV bandgap is in a range easily accessed by lasers, and the magnetic ordering temperature is in a range that readily allows thermal and nonthermal effects to be distinguished.

Time-resolved, second-harmonic generation studies of MnPS₃ were conducted using a range of IR laser energies spanning 0.66 to 1.55 eV to illuminate the sample (referred to as the “pump” pulse) normal to the surface and probed with a second 1.55-eV beam obliquely incident. The experiment was conducted at 10 K, well below the inversion symmetry breaking temperature where second-harmonic generation onsets. The symmetry of the second-harmonic generation effect is studied by rotating the beams and measuring a full 360°.

Two key material properties were coherently controlled in this study: the bandgap and the second-harmonic conversion efficiency. While the sample is transparent to electromagnetic radiation below 0.5 eV and above 1.9 eV. However, electromagnetic waves between those energies traveling through the material still coherently couple to the electronic system and modify it. Adapted from Chu et al. (2020).

Perhaps the most important aspect of this result is that it is a pure quantum control of a solid-state material. Instead of creating excited states in the system, the modifications are fully associated with onsite excitations, and quantum tunneling will cause absorption of light. The bandgap and undergoes magnetic ordering below.

**WAY AHEAD**

This result demonstrates that optical quantum control of some important material properties is possible in certain circumstances and elucidates how it can be done. This paves the way for additional studies of band structure and optical properties control with optical control beams. A tantalizing, but more distant, goal is to extend these protocols to exert coherent control of collective phenomena such as spin and charge ordering. Materials that are insulators, do not have inversion symmetry, and are close to phase transition boundaries such as the trichalcogenides are excellent candidates for such studies to determine to what degree these effects can induced, whether other nonlinear effects can be controlled, and how these effects may be harnessed for novel electro-optic device schemes that do not rely on speed-limiting thermal or electronic modulation.
Dr. James Burgess completed his undergraduate studies at Longwood College, receiving his B.S. in Chemistry. He earned his Ph.D. in Chemistry from Virginia Commonwealth University in 1997 before serving as a postdoctoral research associate at Ames Laboratory, the U.S. Department of Energy’s National Laboratory administered by Iowa State University.

He joined ARO in 2019 following faculty appointments at Case Western Reserve University and Augusta University, where he served as Chair of the Department of Medical, Laboratory, Imaging and Radiologic Sciences in the College of Allied Health Sciences.

SUCCESS STORY

Unraveling the Complex Interactions between Gut Fungi and Bacteria

The first example of gut fungi and gut bacteria interaction at the genetic level has been discovered and characterized. The breakthrough was made possible by tracking gene expression in co-cultures, as previously reported work following biomass degradation missed the interaction. Both the fungi and bacteria exhibit altered gene expression as a consequence of growing in co-culture. Importantly, gut fungi likely produce antimicrobials as a result of competitive existence with gut bacteria. Therefore, gut fungi may be a source of novel antibiotic discovery, a notion of great consequence given the global problem with antibiotic resistance.

CHALLENGE

The human microbiota is infinitely complex, where competitive and symbiotic relationships exist among bacteria, fungi, and viruses; and this soup of microorganisms is also connected to the physiology of the human host, affecting the neurological and immune systems. The microbiota varies between bodily...
locations and between people, especially in different geographic locations. Furthermore, complete genomic characterization of the massive diversity found in one person’s microbiota at one location and at one time is beyond current capabilities. This microbiota is thus a science frontier promising to be rich in discovery of knowledge pertaining to human health and performance.

**ACTION**

The former ICB Program Manager, Dr. Aura Gimm, funded the O’Malley group in 2017 to study fungal–microbial interactions. In 2019, the current ICB Program Manager, Dr. Burgess, met with Professor Michelle O’Malley on the campus of the University of California Santa Barbara (UCSB) for a brief on her research group’s capabilities. Dr. Burgess, being aware of connections between the gut microbial and human performance through the DEVCOM ARL Biology and Biological Sciences Competency, has tracked and collaborated with other ICB actors conducting complementary work in genetic engineering. The development of future, far-reaching biotechnologies, whereby engineered sense-and-respond microorganisms can detect infectious pathogens and produce pharmacologically active molecules to prevent symptomatic disease, will require a basic understanding of the complex interdependencies of fungi, bacteria, and viruses within the human gut microbiome. Dr. Burgess subsequently funded Professor O’Malley’s group in 2021 to conduct work in the area of enzymatic bio-production with Professor Susannah Scott, also at UCSB.

**RESULT**

The O’Malley research team discovered interactions between particular gut bacteria and gut fungi. The team compared isolated cultures of the bacteria and fungi to co-cultures where they were grown together competing for energy. Alterations in gene expression for both the bacteria and fungi occurred when they were co-cultured. Previous work by others following biomass degradation in the cultures missed the bacteria–fungi interaction. The bacteria show an increase in production of drug efflux pumps, while the fungi show activation of their secondary metabolism coupled to production of a defense compound as a consequence of the competitive antagonistic relationship. Taken together, this study suggest that anaerobic gut fungi challenged with bacteria could be a source of new antibiotics. Furthermore, the report demonstrates that the traditional parameters evaluated to discern species interactions are not always adequate and that gene expression factors must be more directly and broadly considered to identify and capitalize on triggered cellular machinery.

**WAY AHEAD**

The research supports the DEVCOM ARL Biology and Biological Sciences Competency. Professor O’Malley is collaborating with DEVCOM ARL intramural researchers by providing strains for fungi so the team can perform joint research on wet waste digestion of anaerobic microbial communities.

**SUCCESS STORY**

**Cell Signaling Aspects of a Mouse Disease State Model Translate to Human Subjects**

The Lauffenburger research group (Massachusetts Institute of Technology [MIT]) used computational methods to uncover biological signatures in a mouse model of Alzheimer’s disease that are also altered in human subjects with the disease. The work represents a significant step forward in the ability to develop hypotheses concerning the root cause of the disease, as well as molecular and signaling pathway targets for pharmaceutical intervention. Overall, such knowledge of the overlap between animal and human disease state biochemistry is needed for efficiency in translating basic science to new treatments.

**CHALLENGE**

Animal and animal cell line studies are often conducted under the assumption that results from such work will allow direct inferences to the human system or disease state. Validation of animal
models as accurate representations of the human cellular singling pathways is a major challenge. Many cellular pathways are found to be altered for a single disease and sorting out cause from effect versus progression of disease is often not currently possible. Documenting animal–human biochemical similarities, especially for disease states, using artificial intelligence (AI)–based computational methods is an emerging tool poised to optimize the translation of basic research to the clinic. More broadly, for enhancement of human performance, human biology needs to be understood in quantitative terms, and studies of analogous animal systems will provide the biological basis for this improved understanding.

**ACTION**

In 2019, the ICB Program Manager, Dr. Burgess, met with Professor Doug Lauffenburger (MIT) at DEVCOM SC in Natick, Massachusetts, and encouraged the submission of a white paper in this area for consideration to be included in the portfolio during the two-year option period of the ICB contract. Based on Dr. Burgess’ technical background involving translation of mouse models of cyclic fibrosis to the human disease state, the critical need for research being conducted by Professor Lauffenburger was appreciated, and Dr. Burgess funded the Lauffenburger group to pursue work broadly described as “interspecies translation via systems biology models.”

**RESULT**

The ICB research team developed an AI platform to measure mouse behavior based on biological pathways inferred from mouse molecular-level measurements that, when combined with parallel human measurements, revealed the biological pathways in mice that were most predictive of human behavior. Figure 2 illustrates the overall computational approach developed for making these critical connections between mice and humans at the molecular level. A novel computational modeling framework, called Translatable Components Regression, is used to translate observations from experimental animals to human subjects. By looking at mouse and human datasets for gene activation and downstream biochemistries together using AI, the team was able to tease out common signaling pathways that would have not been obvious had the datasets been characterized independently. Once identified, it was found that many of these relations are supported by previous published work. Other links between the mouse and human disease state were completely unchartered and will now be the focus of investigation by the broader scientific community. Commonalities between the mouse and human disease states were found in molecular presentations of inflammation in underlying neurodegeneration and immune cell dysregulation.

**WAY AHEAD**

Professor Lauffenburger is collaborating with the U.S. Army Engineer Research and Development Center to pursue neurocognition studies using zebrafish models, for which genetic conservation with respect to humans is significantly lesser than exhibited by rodents or primates. This platform integrates an AI-based approach that supports the DEVCOM ARL Biological and Biotechnology Sciences and Humans in Complex Systems Competencies, and may transition for improved human performance technologies and training as well as treatments for post-traumatic stress disorder (PTSD).
INSTITUTE FOR SOLDIER NANOTECHNOLOGIES (ISN)

Current Scientific Objectives

1. Engages Army colleagues to dramatically improve the survivability and capabilities of Soldiers, their platforms, and their devices by exploring and extending the frontiers of nanotechnology through fundamental research that, if successful, may lead to revolutionary improvements in a wide array of existing equipment and the development of groundbreaking new equipment.

2. With the goal of performing world-class research, engages jointly with Army and industry partners to enable efficient transitioning of research that, if successful, will mature swiftly to the higher technology readiness levels suitable for applied research and development by Army labs, defense corporations, and start-up companies.

SUCCESS STORY

Irreversible 2D Polymerization in Bulk Solution

A DEVCOM ARL-funded ISN team made a breakthrough in 2D polymerization, discovering a once-thought unrealistic method of irreversibly polymerizing in two dimensions in a bulk solution. This finding promises ultra-strong and lightweight polymers with potential uses in ballistics protection, barrier coatings, gas separation, and lightweight structural reinforcements.

CHALLENGE

Two-dimensional polymers only extend in a single plane in units called platelets. However, in a bulk solution, it is difficult to keep them from growing in 3D—a single bond that is formed out of the plane would cause the polymer to grow much faster in 3D than in 2D.

In the past, most researchers have overcome this difficulty by growing polymers along solid templates or fluid interfaces to maintain the dimensionality, or by pre-organizing monomers with reversible reactions, leading to weak bonds that can be broken and reformed before crystallizing them in place. However, these methods are often limited in terms of their stability, scalability, and processability.

A 2D polymer that is made in bulk solution, with irreversible bonds, has been theorized to have high mechanical strength, like graphene, and low densities, synthetic processability, and scalability. Molecular simulations from the ISN team’s DEVCOM ARL collaborators have shown that these materials can achieve previously unattainable films with high mechanical strength per mass and area.

This team realized that there are two potential ways to form 2D polymers in bulk solution: bond planarity and autocatalysis. Bond planarity is the concept that, while most single bonds can easily rotate out of a 2D plane, some double bonds prefer to be planar. Autocatalysis is the idea that already existing 2D polymer structures can act as a template for other platelets to form. This past year, the ISN team set out to discover monomers that could polymerize in 2D in solution (Figure 1).

ACTION

In 2019, Dr. Burgess encouraged an ISN research team to explore new basic science directions in support of shock-mitigating and reinforcing molecular nanocomposites. Dr. Burgess’s proactive leadership of the ISN research program has resulted in the discovery of a new irreversible synthetic scheme.

Figure 1: Synthesis of 2D polymer: (a) Synthetic route to 2D polyaramid, called 2DPA-1. (b) Cross-sectional view of proposed multiple platelet structure. Images courtesy of Professor Michael Strano, Massachusetts Institute of Technology (MIT).
Results

- Published in leading journals to include Science and Nature.
- Discovered irreversible 2D polymerization in bulk solution.
- Generated materials that can be spin-coated into thin films with modulus surpassing unoriented and oriented thermoplastics and cross-linked polymers, with yield strength that is roughly twice that of steel at one-sixth the density.
- Enabled continued collaborative research and development between Army and academic scientists and engineers.

Anticipated Impact

This breakthrough in 2D polymerization promises ultra-strong and lightweight polymers with potential uses in ballistics protection, barrier coatings for corrosion resistance, gas separation, and lightweight structural reinforcements.

Figure 2: Film and fiber properties. (a) A 6-inch 2DPA-1 film on a silicon dioxide (SiO2)/silicon (Si) wafer. (b) 2D elastic modulus and 2D yield strength of 2DPA-1 films of various thicknesses. (c) Schematic of an Archimedean scroll fiber. (d) True stress–strain curves of 2D composite scrolled fibers [data reproduced from Liu et al. (2016)]. Volume fractions: 2DPA-1/PC=7%, Graphene/PC=0.2%. Images courtesy of Professor Michael Strano, MIT.

While their permeability studies are still ongoing, the ISN team’s current data shows an O2 permeability as low as $0.17 \times 10^{-5}$ barrer, which is 36 times lower than that of the most O2 impermeable 1D polymer in literature, poly(ethylene vinyl alcohol) ($6 \times 10^{-5}$ barrer).

These films can be further processed by scrolling them into fiber composites; comparing the properties of a pure PC fiber to one that is 7% 2DPA-1, the modulus increased by 72% and the strength increased from 110 MPa to 185 MPa, meaning that the processed material has great potential for lightweight composites with twice the strength of steel.

WAY AHEAD

A goal of advancing these basic research findings is to create a new generation of lightweight, shock-mitigating materials for protection using this newly identified class of nanostructured polymer. The ISN team plans continued testing and evaluation with its DEVCOM ARL collaborators, Drs. Eric Wetzel and Emil Sandoz-Rosado. Results of these evaluations and collaborations will inform both the DEVCOM ARL the Sciences of Extreme Materials and Terminal Effects Competencies with new concepts for reinforcement and lightweight structural applications. If this testing and evaluation is successful, the 2D polymers may transition toward new classes of lightweight structural materials that enable next-generation DoD shock mitigation materials across the DoD enterprise.

SUCCESS STORY

Thermally Drawn, Integrated Digital Fibers for Advanced Functionalities

An ARO-funded ISN team has created the world’s first programmable fiber, capable of sensing, storing, and analyzing information. These lightweight fibers, when incorporated into a Soldier’s uniform, are able to be programmed for different field applications to collect and make sense of mission-critical data, such as temperature, activity, and heart rate, to improve the Warfighter’s lethality and health in the field.

CHALLENGE

There has never been the ability to program and store algorithms in fibers. The materials required for such digital capabilities (i.e., silicon devices) are not compatible with polymeric fibers. The collaboration between ISN Professors Yoel Fink and John Joannopoulos (MIT) found a way to not only incorporate these digital chips (with sizes much smaller than a grain of rice) into fibers, but also connect thin electrical conducting wires with these chips in the fibers. The connection process between the wires and chips has to be done precisely with only a small margin of error of a few tens of microns—if not, electrical shorting will occur. To add to this difficulty, the connection takes place in a fiber-drawing process, similar to a candy-pulling process. The chips and wires reside in a medium of flowing, molten polymer, highly viscous like honey, which increases the difficulty of precisely controlling the positions of the chips and wires.
The researchers determined the optimal drawing parameters including temperature and tension, and selected a combination of polymeric materials with the physical properties to enable these digital chips to be connected to strands of wires in a highly scalable manner. Up to hundreds of these chips were connected to the electrical wires within the fiber in minutes (Figure 3).

**ACTION**

In 2019, Dr. Burgess sponsored an ISN research team to explore new basic science directions in support of particulate fluid processing for fabric architectures. Building upon past ISN fiber architecture advances with two of the leading ISN fiber expert investigators on the research team, Dr. Burgess led the ISN basic research program such that it has resulted in novel digital fibers that have enabled new concepts such as digital sensing, digital logic, fabric artificial intelligence (AI), and fiber memory capabilities.

**RESULT**

Enabling such digital capabilities in fibers also overcame a major limitation in the field of functional fibers. That is, fibers typically only have a single function per fiber. This work demonstrates multiple functions, including sensing, storing, and analyzing, in a single fiber, with the ability to control each function through a unique digital address. As one thinks about Moore’s law for transistors, this work provides an opportunity for a Moore’s law for fibers, where the number of functions per fiber increases dramatically as the number of transistors per chip increases.

These fibers are also thin and lightweight, can be stranded through a needle (Figure 4), and can be woven into fabrics. When worn on the body, these digital fabrics give insights to what is happening in the human body. The large surface area of skin that the clothing is contacting and the use of fabrics over extended times enable capture of large amounts of data from the human body. Such a digital fabric could give quantitative and qualitative information that reveals previously unknown body patterns.

The ability to program these fibers allows for the storage of machine-learning algorithms and neural networks in the fibers and fabrics themselves. The large amount of data collected by the fabrics increases the prediction accuracy of these fiber-embedded AI algorithms. Such a fabric could operate as an on-body digital assistant to provide real-time analysis and decision-making on the Soldier’s health and day-to-day living, actively alerting the Soldier to any changes in their heartbeat, respiratory health, cognitive health, or sleep cycles. It could autonomously deliver drugs to patients based on their physiological patterns, activate the tired muscles of athletes during training, and alert the wearer to stay hydrated.

**WAY AHEAD**

The ISN team plans to continue to advance the thermally drawn, integrated digital fibers though its partnerships at the DEVCOM SC, MIT’s Lincoln Laboratory, and the Advanced Functional Fabrics of America. This novel approach to digital fibers supports the DEVCOM ARL Military Information Sciences; Network, Cyber, and Computational Sciences; and Humans in Complex Systems Competencies. If these research developments are successful, the digital fiber concepts may transition toward the fiber innovation network to enable a networked military information system relevant to the Warfighter.
Thoughts on ARO: A Unique Gem in the Scientific Ecosystem

Working in an environment and an organizational structure where it seems like things are ever changing around us, I am hoping to remind everyone about what is our constant—what makes ARO unique. Moreover, these are also the things that I value about us, and I hope you do too.

Like the National Science Foundation (NSF), we are an important part of the U.S. science funding ecosystem. Like NSF, we serve a unique niche. And like NSF, we seek to fund the very best scientific research. This should not be too surprising: we grew out of the same early seed, out of Vannevar Bush’s Science—The Endless Frontier report at the end of WWII. But unlike NSF, we are a mission agency, and we have a very important mission: to serve the needs for the future (possibly as yet unborn) Soldier. We serve not even the Soldiers in the next Army, but in the Army after next.

Thus, our hybrid goals embody a tension—a tension between the best science on the one hand, and serving the (largely future, though also the current) Army on the other. This balance, this tension, is what shapes us as a unique organization. (The Office of Naval Research and the Air Force Office of Scientific Research are also unique, having similar but different tensions between basic science and mission. Thus they too play a valuable part in the DoD S&T ecosystem. They are, however, sufficiently different from ARO, so I leave those for another time and another discussion. They are sufficiently similar, however, that coordination and collaboration are essential to avoid redundancy and promote balanced portfolios.)

Because of this precarious balance that we seek, we look for our science to manifest the often evasive concept of “scientific opportunity.” This is something that it feels like we need to define over and over again, particularly as it is frequently misunderstood. It is a powerful organizing principle that helps us pick the best science that simultaneously has the best mission relevance. Without this concept, one can go down endless rabbit holes. For example, we could get pulled too far toward “mission” by crazy ideas like: Wouldn’t it be fantastic if we could avoid all our logistics issues by just teleporting whatever is needed right to the field? Going the other way, we could get pulled too far toward pure science by speculation, looking for the answers to any number of fundamental questions. (As an example, consider the question: Can we discover a magnetic monopole? Maxwell’s equations seem to imply there should be one.) So before going down any such path, we ask questions like: Why now? What is the scientific breakthrough from which we are building? This is what we mean by the “scientific opportunity.” If there turned out to be a “scientific opportunity” for either of these, we might indeed invest in them. The magnetic monopole idea, besides being scientifically interesting, could have multiple DoD applications, such as in multifunctional functional materials; the teleportation idea, if real, might change not only logistics, but also our fundamental concepts of quantum mechanics. Scientific opportunity thus
serves to keep us focused on what’s real while simultaneously keeping us on the cutting edge of where the science currently is.

Besides a balance between the best science and the mission, as already discussed, there is also the balance between near-term mission and “the Army-after-next”—the latter being an essential and unique mission. This balance means that ARO will certainly help solve the near-term problems that require basic research, but that we mustn’t lose sight of our founding mission—the mission that no one else in Army or anywhere else serves—to look out for the future Soldier. This is the aspect that makes ARO unique—something we must remember amid pushes toward “relevance.” Our mission is indeed relevant for the Soldier, but the future Soldier is easily overlooked in the crunch of needs for the present-day Soldier.

In seeking to find “scientific opportunity,” both we and the scientists we fund must know what’s “out there” scientifically, encompassing ideas from wherever they might arise. This is why it is critical to find the interconnections of different ideas, often spanning disciplines, but even within the same discipline, spanning concepts and history (e.g., putting together something long forgotten or merely something that was until now of idle curiosity, which, when combined with something recently discovered, can make a breakthrough). This is why having the most eyes possible (with the most different perspectives) on the work is of critical importance.

Having many eyes and many perspectives on an idea is critical, but it is very difficult for us in the United States today, with a limited population interested in pursuing science and engineering (S&E). Our historical solutions have been to attract new people, whether to entice more students into science, technology, engineering, and mathematics (STEM) or to attract the many foreign students that come to the United States to study in our universities and then stay after graduation. Educational innovation only goes so far to attract traditional new U.S. students, limiting the reach of this first option. However, attracting underrepresented minorities (URMs) has far greater potential if it can be done successfully. The second option, attracting and retaining foreign students, is limited by growing xenophobia combined with foreign universities having learned from and emulating our schools to such a degree that there are now many more attractive choices for foreign students. These two options—increasing the U.S. STEM pipeline or competing more effectively to attract and retain foreign scientists to remain in the United States—are critical to domestically cultivating scientific advances by ensuring that we have the greatest number and most diverse possible eyes on scientific ideas.

Increasing the reach of STEM in the United States seems hopeless if we consider only the traditional demographics. For example, we will never have the sheer number of potential S&E students as a country as large as China—they are on track to have in the not too distant future more S&E students than the United States has students in total. But we do have an almost untapped reservoir of students who we have historically pushed away. Most of these URMs are currently close to negligible in their representation in the S&E workforce (percentages are barely in the single digits). Women are slightly better represented, but still at levels that are far from satisfactory. Why is this? Despite decades of trying to remedy this situation and periodic pushes to “do better,” little has changed. In fact, in some disciplines, there is evidence that things have actually become worse in the past decade or so. There is now active research focused on understanding the underlying causes, a field that appears to be making progress, and which, if successful, could be used to institute remedies. This is one direction of hope.

Going back to the second option, enticing our foreign students to stay in the United States needs to be another focus. Our national policies unfortunately work against us in this regard. One hope is to look beyond students, to science internationally for those “other eyes.” In other words, perhaps some of this need can be made up for by increases in our foreign collaborators. This is a potentially even larger pool. We need to keep in mind that science is an international enterprise. We should not forget the lessons from WWII, where different pieces of knowledge crucial for the war effort and for our final victory came from scientists from around the world. Putting together disparate pieces and making interconnections was, and is, critical. International engagement remains key.

But hasn’t our situation changed? We have adversaries who act unscrupulously and take advantage of our research. How do we protect ourselves? Research protection is indeed important. Historically, let us not forget that research protection was critical during WWII and also during the Cold War period afterward. This period marked the origin of much of our current regime of protections, which are grounded in classification. Nuclear secrets posed a highly existential threat. As the Cold War got its closest to heating up, a fierce debate raged in the Reagan years about how to protect America’s S&T. The upshot, embodied in NSDD-189, which still stands today, determined that basic 6.1 science is not classifiable because the benefits we gain to the development of scientific ideas and concepts in an open global research ecology greatly outweigh the risks—at least until one gets to the space of...
Applications. This established the national policy for controlling the flow of scientific, technical, and engineering information produced in federally funded fundamental research at colleges, universities, and laboratories. Specifically, NSDD-189 states that “the conduct and informational products of fundamental research are to be unfettered by deemed export restrictions.” It was not until at least the 6.2 level that research could be considered for classification. This view was recently affirmed by the National Science Board’s statement on science and security that “strongly reaffirms the principle behind President Reagan’s National Security Decision Directive 189 (NSDD-189): ‘our leadership position in science and technology is an essential element in our economic and physical security. The strength of American science requires a research environment conducive to creativity, an environment in which the free exchange of ideas is a vital component.’”

We need to work within a global scientific ecosystem where we aren’t the only ones producing ideas and innovation. In fact, the world largely learned that from us over the past decades.

This view is being actively debated in policy circles right now. I believe NSDD-189 has it basically right. We aren’t the only smart people in the world. We need to work within a global scientific ecosystem where we aren’t the only ones producing ideas and innovation. In fact, the world largely learned that from us over the past decades. Many countries now have thought-out national policy for investing in S&T and enhancing their higher education; importantly, these policies include global foreign investments and collaborations. This is enabling adversaries to rapidly improve defense-related R&D advances. As a result, what we need to do, I believe, is more subtle and within the guidance of NSDD-189. For example, as a consequence of national directives from Congress and the President, we are now considering how to prevent our research from finding its way to an adversary. We are asking: Should we fund research that might benefit an adversary? Taking such steps is wise. In this process, however, we must be vigilant that the steps we take do not restrict the set of eyes and minds on a basic scientific concept before it becomes a technology. While bad behavior on the part of our adversaries can pretty much be counted on, we don’t want to implement “solutions” that might in the end harm us more than help us. By taking DoD funding out of the loop, we would not prevent the work from being done—but we might eliminate our ability to shape it and adapt it as readily.

The scientific process is nonlinear, going back and forth between ideas in disparate fields, from disparate times in history, and even from science to technology. Examples of the latter are widespread, but a highly salient example is that it took the invention of the laser to enable most scientific innovations in chemistry, physics, and even materials science that have been realized over the past few decades.

We often hear talk about speeding up the process of science. Ideas develop by the types and variety of interconnections that are made across scientists and disciplines, as described previously. “Speeding up” science is not something that can magically be done by changing some “process” by which science is done. Instead, we need the maximal engagement of minds with varying perspectives to take part in the evolving science. Hence, the need already described for more URMs, foreign students, and international collaborators is evident. Unfettered research protection carries the risk of slowing down the pace of our own progress and of our own scientific advances.

Moreover, framing the problem so far has been from a U.S.-centric perspective. This may have been excusable a few decades ago, but these days many discoveries do not start in the United States. We have to accept that in many areas we no longer lead. For example, though ultra-cold atomic matter is a research field that clearly originated from U.S.-based research of the 1970s and 80s, many of the discoveries are no longer ours. In 2019, the decades-long-sought supersolid phase of matter was discovered in material systems—namely, in dipolar quantum gases, Bose-Einstein condensates (BECs) in particular. Half a century ago, researchers predicted supersolidity, an intriguing phase of matter that combines the frictionless flow of a superfluid and the crystalline structure of a solid. The prediction sparked an intense experimental quest to find a supersolid. The three recent papers that nearly simultaneously reported supersolidity were published by researchers at the University of Innsbruck, in Austria, and at the University of Stuttgart, in Germany. Even what such a phase might “look like” was controversial, as it is truly counterintuitive to be both solid and fluid at once. In dipolar BECs, attractive short-range interactions and long-range dipolar forces between the atoms compete, and cause spontaneous clumping of superfluid droplets into crystalline structures. These dipolar supersolids offer flexible and controlled experimental platforms for studying supersolidity, allowing for systematic studies of the counterintuitive properties of these exotic states of matter. The United States is actively engaged in exploiting this new phase of matter, both for potential applications and to deepen our understanding of quantum phases and quantum materials generally. This example shows how critical it is for international-based research to reach us.

This work stems from work in allied countries. But purely scientific work emanates from everywhere and benefits all. In 2015, researchers in China discovered analogs of Weyl fermions—massless, chiral particles predicted by quantum field theory—in solids whose electronic bands cross at “Weyl nodes”
near the Fermi surface. The discovery papers were by researchers at the Chinese Academy of Sciences (CAS), who found Weyl fermions in tantalum arsenide (TaAs). Another research group at CAS laid the foundations for the discovery. Their theoretical calculations suggested that a family of nonmagnetic materials including TaAs was a promising target for spotting these quasiparticles. After the discovery, yet another group at CAS reported measurements of the “chiral-anomaly” property of Weyl fermions, confirming a predicted imbalance of the handedness, or chirality, of the quasiparticles when the material is subjected to certain electric and magnetic fields. The discovery of Weyl semimetals has spurred tremendous interest in topological semimetals and led to the discovery of many other exotic materials world-wide, not the least of which effort is in the US. The research field is vibrant, with extensive efforts now ongoing, including by ARO-funded researchers, to further understand this class of topological materials and harness the materials’ properties in devices. Without the initial set of research ideas from China, we would not have arrived at this place.

An example perhaps closer to technology, and in fact an area of great concern in our current competition, is hypersonics. One of the greatest challenges for this field is overcoming the aerodynamic heating resulting from hypersonic flows. The temperature of the air passing over a vehicle going near Mach 5 has been measured to be over 2000 K. The inevitable onset of turbulence at high speeds contributes greatly. But surprisingly, strong heating also occurs in laminar flow. That there is a separate aerodynamic interaction that causes this was identified fairly recently by researchers at China’s Peking University. In fact, their work also showed how this interaction could be tuned to result in cooling rather than heating. This is a critical insight and one that might surprise us coming from a competitor.

Hopefully these examples make it clear that, on the one hand, we gain by science being open and on the other hand, we need to be prepared to build on results such as these as soon as they occur. Certainly a lesson from this is that our Army and DoD S&Es must be on top of the international science, as progress like this can and does occur everywhere. And ARO’s real advantage will come from all of us staying at the top of our expertise in our fields and being able to spot the advances (and specifically the scientific opportunities) faster than our adversaries.

To again quote NSDD-189, “[T]he strength of American science requires a research environment conducive to creativity, an environment in which the free exchange of ideas is a vital component.” ARO plays a key role in ensuring the strength of scientific creativity employed for the advantage of the U.S. Army. We must continue to balance among the competition of scientific creativity, Army need, and national security.

As prefaced, these are my thoughts on the strengths of ARO and DoD science, and the funding ecosystem that we are part of. Along the way, I indirectly posed some questions to think about: What is the right balance among the competing needs? How do we know if we have it right? Not posed, but worth thinking about since we are scientists, is there a scientific way to address these questions? I think this last question could itself open an interesting discussion.

“Speeding up” science is not something that can magically be done by changing some “process” by which science is done. Instead, we need the maximal engagement of minds with varying perspectives to take part in the evolving science.

ARO plays a key role in ensuring the strength of scientific creativity employed for the advantage of the U.S. Army. We must continue to balance among the competition of scientific creativity, Army need, and national security.
Chapter 4
ARO Active MURIs

This chapter provides a brief summary of all ARO MURIs that were active in FY21, organized according to the year the MURI began. Each MURI is driving fundamental studies that will also impact one or more of the ARL Competencies, as indicated in the following table.

This background image is from success story “p53 Overexpression Induces the Formation of Stable Prion Aggregates” on page 168.
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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 FY21

Anomalous DipoleTextures in Engineered Ferroelectric Materials

The goal of this MURI is to develop a theoretical understanding of anomalous dipole textures in ferroelectric materials and experimentally study their creation, dynamics, interactions, and annihilation in advanced materials.

This MURI began in FY21 and was awarded to two teams. One team is led by Professor Ramamoorthy Ramesh, University of California, Berkeley. The objective of this MURI project is to develop an understanding of polarization topologies in thin films and superlattices with atomic-scale perfection such that competing energy scales can be produced to the formation of emergent phenomena. In this project, the MURI team proposes to bring together a comprehensive combination of first-principles-based atomistic simulations, phase-field modeling, thin-film synthesis, and advanced characterization methodologies to both predict and realize exotic dipolar textures such as polar vortices and skyrmions. Mainly, the team will focus on addressing three thrust areas: (1) discovering new ground states and expanding control of those states with a focus on identifying and confirming topologically nontrivial natures and novel phase transitions; (2) demonstrating control via applied stimuli to the emergent polar structures with initial efforts centered on electric-field control of vortex and skyrmion permittivity, electromechanical response, dynamics, and chirality; and (3) expanding the scope of superlattice structures to bring about additional emergent functions with special attention to developing spin-charge coupling at the atomic scale. If successful, this effort could provide unprecedented pathways to the creation of novel topologies in ferroelectric and magnetic systems with deterministic control in response to applied electric, magnetic, and stress fields; light; temperature; etc. The new materials and understanding would enable the development of novel applications in next-generation logic, memory, sensing, and field-tunable, high-frequency applications such as phased array radars, etc., in support of the Network C3/I and Soldier Lethality Army Modernization Priorities.

A second team is led by Jayakanth Ravichandran, University of Southern California. The objective of this project is to probe inherent polar textures in quasi-1D hexagonal chalcogenides and induced polar textures due to proximity effects in heterostructures of quasi-1D hexagonal chalcogenides with other perovskite chalcogenides, 2D materials, and single-crystalline oxide layers to elucidate the mechanisms to introduce polar textures in active electronic materials. The MURI team proposes three thrusts: (1) use density functional theory and phenomenological modeling to develop mechanisms to interface polar textures and electronic materials, with a focus on understanding the mechanism of anomalous polar textures specific to model systems such as barium titanium sulfide (BaTiS3)-based heterostructures; and (2) discover synthesis and fabrication methods to achieve large single crystals of BaTiS3, epitaxial heterostructures of BaTiS3 by direct growth, and transfer printing to form heterostructures for the studies in Thrust 3 and characterize associated structural, chemical, optical, and electrical properties, including room-temperature and low-temperature electron microscopy studies to probe the nature and evolution of polar textures in BaTiS3 and its heterostructures; and (3) studying the creation, destruction, and manipulation of polar textures and their properties using (a) scanning tunneling microscopy at room and cryogenic temperature to understand the atomic-scale structures, (b) piezo force microscopy at room temperature to understand the microscopic polarization, and (c) ultrafast spectroscopy to understand the nature and origin of the anomalous textures in the bulk and surface of BaTiS3 and its heterostructures. This work aligns well with the Intelligence functional concept and would help to create high-density memory devices in the future and supports the Army Modernization Priority of Network C3/I.
Cyber Autonomy through Robust Learning and Effective Human–Bot Teaming

The goal of this MURI topic is to obtain scientific understandings and establish models for trusted cyber autonomous systems that support robust learning (especially from failures), exhibit anti-fragility adaptation, and allow cyber bots teaming among themselves or with human agents in order to achieve mission assurance under highly dynamic and adverse environments.

This MURI began in FY21 and was awarded to two teams. One team is led by Professor Somesh Jha, University of Wisconsin–Madison. One of the greatest cybersecurity challenges today is successful coordination among human–bot teams—as failure to coordinate can have disastrous consequences in the cyber battlefield. Unfortunately, while we know a lot about how humans use tools to work in teams, little is known about how to manage, observe, and improve hybrid teams of humans and bots. This project focuses on teams engaged in cybersecurity tasks or cybersecurity teams, such as threat intelligence and cyber defense. The MURI project brings together a team of eight U.S. and eight Australian principal investigators (PIs) with diverse expertise spanning computer security, machine learning (ML), psychology, decision sciences, and human–computer interaction. The project will carry out research in the following five research thrusts: (1) analyst-friendly and task-driven explanations, (2) robustness, (3) building human–machine shared models, (4) robustness and anti-fragility at the team level, and (5) verifying cognitive–machine models.

A second team is led by Professor Farinaz Koushanfar, University of California, San Diego. This project introduces a novel multi-pronged approach to address the standing challenges for future warfare involving a multitude of cyber bots. Important constraints in bot warfare scenarios include limited access to a reliable central controller, speed of action, synchronization, and coordination among the distributed cyber-physical, cyber, and human entities. The interdisciplinary team of PIs aims to develop a new comprehensive foundational framework for safe and robust artificial intelligence (AI) intrinsic to autonomous agents, distributed bots, self-adaptivity, introspection, and human–AI teaming, as well as automated methods for human–AI games, deception, and recovery in dynamic settings. The focus of the research is on three modular but inter-linked thrusts. (1) Robust learning: The team will formulate key challenging scenarios in robust learning with distributed agents as instances of graph optimization problems; the formulation is leveraged to derive new bounds, metrics, attacks, and defenses. (2) Introspection/anti-fragility adaptation: This is formulated as active learning scenarios with offline preprocessing and training, online introspection/anti-fragility adaptation, and dynamic adversary deception. (3) New team science concepts for cyber bots: This thrust will focus on effective team assembly, shared cognition for human–AI interaction, quantifying performances over time and tasks, robust team training by reinforcement learning (RL), robustness to low-probability high-impact events, and self-adaptive mixed initiatives control and deception.

Understanding and Engineering Transient Mechanical Responses in Nanoparticle-Reinforced Heterogeneous Particulate Systems

The goal of this MURI topic is to determine how fine-particle interactions create a macroscale metastructure in systems containing a mixture of fine and inert coarser particles accurately describe the structural influence and, from that knowledge, develop both constitutive models based on a mechanistic understanding that predict the macroscale behavior of these highly heterogeneous particle systems and processing methods for the inducement of desired metacrostructures via rheological, electrostatic, chemical, or alternative mechanisms.

This MURI began in FY21 and was awarded to a team led by Professor Jennifer Lewis, Harvard University. Highly heterogeneous mixtures of attractive fine and inert coarse particles exhibit a rich array of behavior in response to mechanical loading. The MURI team aims to understand the reversible transition between solid and flowing states in systems with high solids loading and variable moisture content, which is crucial for applications ranging from soils with engineered stress–strain–time response to novel particulate inks for additive manufacturing that withstand slumping or deformation under self-weight. To achieve the overarching goal, the team is conducting a tightly integrated program of research that combines multiscale modeling, geotechnical and rheological measurements, 4D imaging, and microscopic theory focused on nanoparticle-reinforced granular mixtures. The research efforts are divided into two major thrusts: (1) multiscale theoretical and computational modeling of highly heterogeneous particulate
systems and (2) foundational experiments to elucidate their transient behavior and structural evolution under mechanical load, which will be exploited to create new classes of engineered soils and printable inks with novel properties. The primary outcome of these efforts will be to establish a predictive multiscale, multi-physics framework, validated by experiment, for engineering highly heterogeneous particle systems via tunable interactions that arise within nanoparticle-reinforced granular networks. This work is related to engineered soils, with expected applications to infrastructure, mobility, and airfields, as well as for metastructured inks for 3D printing of critical interest for Army and DoD applications. The effort is a Cooperative Agreement with AFRL and ERDC’s Construction Engineering Research Laboratory.

### Novel Mechanisms of Neuro-Glio Bio-Computation and Reinforcement Learning

This goal of this MURI is a combined effort of advancing the theory for RL systems and advancing the neurobiology of astrocytic function through a synergistic design of theory and experiments in humans and animals. Deep RL has enabled superhuman performance in challenging video games and control tasks, and particularly in games with perfect knowledge and deep search (Go, chess). RL is also a key framework to model and understand how neural circuits acquire complex functions as a result of time and experience. However, there remains a significant gap between the often slow, fragile, and computationally demanding performance of artificial systems and the fast, robust, and efficient learning exhibited by animals and humans.

This MURI began in FY21 and was awarded to two teams. One team is led by Professor Mriganka Sur, Massachusetts Institute of Technology (MIT). To address this challenge, they will build a new theoretical framework for RL based on a theory of potential-based methods. By separating value estimation from action selection, and integrating costs and benefits across time, the theory naturally solves the exploration–exploitation dilemma and enables mapping its predictions to the functional anatomy of brain structures, including the prefrontal cortex (PFC) and striatum. Importantly, preferential innervation of the PFC by the neuromodulator norepinephrine and of the striatum by dopamine represent important mechanisms for selectively activating astrocytes and modulating task-specific neuronal output. The theory thus relates to the architecture of neuron-glia interactions in the brain, which will formalize with a new class of networks, Glial Deep Neural Networks.

A second team is led by Professor ShiNung Ching, Washington University in Saint Louis. The overall goal of this project is to construct new RL-ML methods that obviate existing challenges by validating a novel theory of neurobiological learning based on the dynamical interactions of neurons and astrocytes, a key type of glial cell. Despite their ubiquity in the brain, the functional role of glia is poorly understood. The central hypothesis is that astrocytes and neurons form two levels of a coherent, reciprocally connected hierarchical network where astrocytes integrate contextual information and modulate neural circuitry in a manner favorable for large-scale learning. The research team postulates that neuronal and synaptic processes can be rapidly influenced by astrocytes, allowing learning to occur quickly when task circumstances change and for prior contextual information to optimally constrain learning when new requirements are faced.

### Quantum Network Science

The goal of this MURI topic is to define and develop the nascent field of quantum network science through a combination of theoretical investigations spanning from fundamental axiomatic studies to the development of algorithms and mathematical tools, and of experimental verification of theoretical predictions. These tools will be used to demonstrate robust, high-capacity, and fundamentally secure quantum-classical networks in architectures enabling entanglement distribution and distributed quantum information processing (QIP).

This MURI began in FY21 and was awarded to two teams. One team is led by Professor Saikat Guha, University of Arizona. The MURI team plans to achieve this objective by working through four primary tasks. In Task 1, they will pursue an axiomatic development of fundamental quantitative measures and associated scaling laws for multi-site, multi-qubit entanglement, where the intuitively formulated axioms may target specific properties the entangled network should possess. In Task 2, they will develop new mathematical tools and algorithms to study the generation, distribution, evolution, manipulation, and control of networked entanglement.
In Task 3, the team will take a broad look at applications of quantum networks at all scales—viz., a network of qubits within a computer, network of computers, and network of networks—focusing on what new insights are afforded by a network science study. Finally, in Task 4, the team will build an experimental platform, a universal-quantum-logic-capable quantum network emulator of color-center qubits with long coherence times and a reconfigurable connectivity. The emulator will be used to verify their theoretical predictions and serve as a research tool to advance quantum network science, as classical simulations of quantum networks will not scale.

A second team is led by Professor Chee Wei Wong, University of California, Los Angeles. This MURI team seeks to pair leading-edge network science and protocols with quantum networks in a tight synergistic partnership among network scientists, quantum information theorists and physicists, and experimental test bed validation. The MURI work comprises four interrelated thrusts: (1) network science and percolation for robust network entanglement distribution; (2) transformative protocols with high-dimensional, multi-partite quantum states for high-capacity network links and functionality; (3) distributed quantum network processing and validation testbeds including algorithms and protocols; and (4) cross-disciplinary foundations and mathematics for frontier quantum networks, including network classical-quantum coding bounds, quantum network information theory, and multi-partite graph states for robust quantum networks.

Multifunctional Devices in Precisely Engineered van der Waals Homojunctions

The goal of this MURI topic is to integrate dissimilar electronic phases of matter in any individual 2D material through geometric tiling and stacking along with external fields to reveal emergent electronic thermal and/or optical phenomena and design functional device concepts based on them.

This MURI began in FY21 and was awarded to Professor Philip Kim, Harvard University. The objective of the MURI team is to create functional interfaces in single 2D van der Waals (vdW) homojunctions, through which quantum emergent phenomena and their application in novel devices concepts will be pursued. The team is developing novel functional vdW homojunctions—structures that will realize the integration of multiple phases in electronic, optoelectronic, plasmonic, and quantum device applications. Atomically sharp homostructures in a 2D material will exhibit a wide variety of interfacial properties that are not constrained by chemical and lattice mismatch. Relative twist between layers and lattice mismatch-induced strain will produce a moiré superlattice, to achieve nanometer-scale band structure engineering. The MURI teams is pursuing these goals in three 2D vdW material platforms: graphene, tungsten diselenide (WSe₂), and tungsten ditelluride (WTe₂). Integration methods seek vertical and lateral stacking in a controlled environment in a materials-agnostic approach. The materials and structures will be probed by a series of experimental tools to characterize the engineered vdW structures, in close collaboration with theory, for efficient feedback through ML methods. Device concepts include (1) combined plasmonic and hydrodynamic behavior for terahertz (THz) emitters and (2) entangled photon and Cooper pair quantum devices.

Tunable III-Nitride Nanostructures for N≡N and C-H Bond Activation

The goal of this MURI topic is to develop and understand the behavior of Group 2 nitrate semiconductor photoelectrocatalysts with a tunable energy bandgap in the visible and near-IR wavelength range and explore their structural, surface electronic, and photocatalytic properties.

This MURI began in FY21 and was awarded to Professor Zetian Mi, University of Michigan. The MURI team will provide a comprehensive theoretical and experimental understanding of dilute anion III-N nanostructures (Ga(In)NX) for N≡N and C-H bond activation. This will be accomplished through multiple cycles of an iterative approach where computational design of materials with desired optical, electronic, and reactivity properties will identify promising surfaces, dopants, and co-catalysts, guiding the synthesis of spectrally tunable Ga(In)NX nanostructures, and spectroscopic characterization of carrier dynamics and catalytic reactivity. State-of-the-art epitaxy and surface functionalization by atomically dispersed active sites will provide high-quality photocatalytic platforms. Fundamental studies will characterize the unique structural, optical, electronic, and photocatalytic properties enabled by these novel
ACTIVE MURIS THAT BEGAN IN FY20

Adaptive and Adversarial Machine Learning

The goal of this MURI topic is to build adaptive ML systems that are capable of performing against corrupted training data, evasion attacks, and unexpected inputs. Achieving these goals requires mathematical and algorithmic development frameworks that are application- and implementation technique-independent. This framework should enable the development of robust and adaptive ML-based intelligent systems, with predictable properties and performance bounds that are capable of generalizing, reflecting, and reasoning in a contextual manner.

This MURI began in FY20 and was awarded to a team led by Professor Insup Lee, University of Pennsylvania. The objective of Professor Lee’s effort is to develop the foundations for robust and adaptive learning based on childhood development. This will be achieved over three phases: (1) concept-based learning robust to adversarial examples, (2) adaptive learning in dynamic environments, and (3) verification and monitoring of learning. The approach will utilize concepts (e.g., prior models and shapes) inherent in the physical world, while simultaneously detecting and adapting to changes in the environment and concepts, such that robustness claims can be validated through a combination of offline verification and runtime monitoring. Evaluations of the techniques will be performed on an interactive robotic platform as a surrogate for future military applications involving cooperative robotic systems with learning in a battlefield environment.

Axion Electrodynamics beyond Maxwell’s Equations

The goal of this MURI topic is to develop a new class of electric-field tunable axion device concepts such as electric-field switching of ferromagnets, voltage tunable magnetic inductors, filters, resonators, and non-reciprocal devices without current dissipation through a cohesive, multidisciplinary approach involving electronics, physics, and materials. This research will focus on the formation of pristine, atomic-level interfaces between (known) topological materials and non-topological materials; the physics of the intertwined electronic and magnetic phenomena amid electrical contacts and other media necessary in a real, non-idealized environment; and techniques for observing and exploiting the axion term for unique magnetoelectric effects in these heterostructures. In other words, the aim is to fundamentally understand axion electrodynamics in topological solid-state systems and demonstrate axion-based electric-field control of both electric and magnetic properties.

This MURI began in FY20 and was awarded to a team led by Professor Norman Peter Armitage, Johns Hopkins University. The objective of Professor Armitage’s effort is to exploit the novel “axion” magnetoelectric response of topological materials—including magnetic topological insulators and Weyl semimetals—to generate new routes to couple electric and magnetic degrees of freedom in materials and devices. This will be achieved by combining state-of-the-art materials development, device fabrication, THz spectroscopy, analytical theory, electromagnetic (EM) modeling, nonlinear optics, and local probes of EM response to elucidate fundamental aspects of the axion response in topological systems. By focusing on axion electrodynamics, ultimately, this research has the potential to unlock high-performance materials and devices capable of room-temperature operation of broad interest to both academic and DoD communities.

Engineering Endosymbionts to Produce Novel Functional Materials

The goal of this MURI topic is to leverage recent advances in materials science and synthetic biology to develop a eukaryotic organism driven by a programmable prokaryotic organism and use the hybrid system to explore the creation of novel functional materials. Eukaryotic systems provide opportunities to realize more sophisticated products; however, these complex organisms present significant challenges to engineer and program. In a hybrid system, the best of both can be
achieved: an engineered, prokaryotic endosymbiont controlling a eukaryotic host cell to produce materials of interest. This project will explore the fundamental process of biosynthetic production of novel functional materials using a eukaryotic organism controlled by a more easily and rapidly engineered prokaryotic endosymbiont for rapid, flexible, modular control.

This MURI began in FY20 and was awarded to a team led by Professor Jeffrey Barrick, University of Texas at Austin. To address this challenge, Professor Barrick proposed to genetically engineer bacterial endosymbionts that live within the bodies of animals or plants into onboard control modules and molecular factories that enhance the production and properties of the biomaterials. Specifically, they will develop and demonstrate these transformational capabilities by engineering endosymbionts that enhance brochosomes—natural nanostructures with novel surface and optical properties that are produced by leafhopper insects. If successful, this research will address a longstanding, unsolved challenge in the ability to engineer hybrid systems whereby a prokaryotic endosymbiont controls a eukaryotic host cell to produce materials of interest, ultimately leading to a broad range of disruptive technologies having significant impact on DoD capabilities.

**Information Exchange Network Dynamics**

Recently observed differences between the propagation of legitimate and misleading news items in social media have made it necessary to revisit traditional models of information dynamics over networks. The goal of this MURI topic is to model the dynamics of cognitive processes over information networks for efficient information diffusion, controlling its veracity and forecasting potential cognitive outcomes of these dynamics. Achieving this goal requires leveraging recent advancements in experimental psychology, computer science, and information theory to enable understanding of information flow dynamics.

This MURI began in FY20 and was awarded to a team led by Professor Cedric Langbort, University of Illinois at Urbana-Champaign. To address this challenge, Professor Langbort will establish an understanding of the multimodal dynamics of information over networks by developing rigorous models of such multimodal information transmission that explicitly account for intentionality and capturing the effects of psycho-cognitive factors. More specifically, Professor Langbort proposes a multidisciplinary approach to address three interconnected research themes: (1) the development of models of intentional information transmission on networks, (2) their enrichment to incorporate behavioral elements such as lack of rationality and Bayesianity and the role of emotions, and (3) their validation in experiments and on preexisting datasets. This framework should enable the development of models that can determine how authentic information and misinformation are propagated differently, and devise ways to quantify misinformation spreading.

**Mathematical Intelligence: Machines with More Fundamental Capabilities**

Construction of error-free programs is empirically difficult, and error rates increase in line with their complexity. To overcome this challenge, experts are beginning to recognize that error-proof, machine-generated programming is mandatory when zero tolerance in execution is required. The goal of this MURI topic is to develop the new science of iteratively constructed logical deduction in the context of quantum field theories (non-relativistic, relativistic, and topological) for QIP and develop its basis as a foundation for certifiable automated reasoning. This will ultimately enable mathematically intelligent (MI) machines equipped with deduction, induction, and logical inference, capable of generating new insights that are certifiably correct.

This MURI began in FY20 and was awarded to a team led by Professor Arthur Jaffe, Harvard University. To address this challenge, Professor Jaffe proposes to investigate protocols, algorithms, complexity, error correction, and the certifiability of quantum processes using mathematical insights that combine picture calculus, quantum logic, and quantum field theory. By linking extremely abstract, theoretical ideas with practical laboratory implementation, the MURI team hopes to provide a rigorous theory for MI machines, ultimately enabling the construction of a quantum computer that can substantially improve present error correction codes.

**Quantum State Engineering for Enhanced Metrology**

Assured position, navigation, and timing is a high priority, especially for autonomous platforms. For platforms to maintain accurate knowledge of their position, orientation, and altitude during missions, the uncertainty errors accumulated over time have to be constrained by external aides. Quantum systems are a promising candidate to aid in minimizing uncertainty due to their
demonstrated position. Two important questions about quantum sensors remain: (1) Can special quantum states be realized that push the performance of these sensors to the fundamental limit? and (2) Can these systems be engineered such that their exquisite sensitivity is constrained to what one intends to measure? The goal of this MURI topic is to investigate these knowledge gaps and develop methods that explore quantum correlations and special states to enhance metrology, improve sensitivity, achieve fundamental uncertainty limits in different ways, and integrate these states with thermal reservoirs and strong system design to mitigate decoherence.

This MURI began in FY20 and was awarded to a team led by Professor Monika Schleier-Smith, Stanford University. To address this challenge, Professor Schleier-Smith proposes to develop protocols for generating metrologically powerful entangled states that are robust to develop real-world noise and realistic experimental imperfections to explore how resilient entanglement is in the real world. By comparing idealized experiments to disordered solid-state platforms, the MURI team will develop the tools necessary to transfer techniques from well-controlled academic labs to the field. The techniques will enable next-generation atomic clocks with world-leading, short-term stability and robustness to noise. Ultimately, this effort will result in a clear assessment of when entanglement provides a practical win for real-world sensors, and a roadmap of algorithms and platforms necessary to make such sensors a reality.

**Solution Electrochemistry without Electrodes**

Traditionally, electrochemistry is focused on a system where electron transfer occurs at an electrode surface. In these systems, the electroactive species interacts with the electrode and this interaction has an effect on electron transfer. Recent advancements in the surface plasmon decay of metallic nanoparticles coupled with light and atmospheric plasmas have been used to generate electrons, indicating that non-electrode electrochemistry is feasible. However, to date, very little research has been dedicated to using surface plasmon-based systems to drive solution electrochemical reactions. The goal of this MURI topic is to explore and understand the electrochemistry between electrons that have been generated by methods such as atmospheric plasma, surface plasmon, or pulsed radiolysis and solution species. This effort is focused not only on controlling the generation of electrons, but also the characterization of their energies and lifetimes including electron penetration and diffusion to solution species, as well as novel solution electrochemistry and electrosynthesis.

This MURI began in FY20 and was awarded to a team led by Professor Peter Bruggeman, University of Minnesota, Twin Cities. To address this challenge, Professor Bruggeman proposes to investigate foundational scientific questions addressing plasma-induced species in solutions and their role in chemical transformation. This will be achieved by exploiting recent advancements in pulsed power and radio frequency plasmas to enable unprecedented controllable injection of electrons into solution on nanosecond timescales commensurate with the typical lifetime of reactive intermediates in solution. The resulting improved control of electron and ion fluxes and energies incident into the solution will enable synthesis of nanoparticles and polymers with desired but previously uncontrollable or unattainable properties.

**Stimuli-Responsive Mechanical Metamaterials**

Metamaterials research has categorically demonstrated the potential for microarchitected materials to surpass the intrinsic properties and functionality of natural and conventional materials. Notable advances in chemical triggering mechanisms and nanomaterial assembly has opened doors to fabricating stimuli-responsive mechanical metamaterials with unprecedented architectural control. However, realizing the utmost potential for rationally designed active metamaterials requires research on the role of interfacial phases as well as pathways for integrating modern understanding of metamaterial wave dynamics and topological mechanics. To fully realize the potential of responsive metamaterials, this MURI is focused on creating stimuli-responsive mechanical metamaterials with precise nanoscale interparticle, interfacial, and functional control.

This MURI began in FY20 and was awarded to a team led by Professor Nicholas Boechler, University of California, San Diego. To address this challenge, Professor Boechler proposes to investigate the fundamental structure–activity relationships that govern the interplay of metamaterial mechanics and changes in the properties of the primary constituent material. More specifically, the MURI team will target challenges at the intersection of metamaterials and stimuli-responsive materials including the slow active response in metamaterials with stimuli-responsive constituent materials, the one-way response of stimuli-responsive constituent materials, and the application of these topological
mechanics at micro- to sub-nanoscales. This will be achieved by pursuing a series of experiments where the responsive chemistries employed act as chemical triggers that will initiate chemical signals in the form of electrons and protons, which will induce a material response in the form of change in modulus, shape, or addition/removal of material. These advances will lead to new types of metamaterials that have unprecedented capabilities for energetic transformation and wave control, ultimately informing the design of DoD-relevant stimuli responsive material systems.

ACTIVE MURIS THAT BEGAN IN FY19

How Sleep Clears Your Brain: Slow Waves, Glymphatic Waste Removal, and Synaptic Down-Selection

This MURI began in FY19 and was awarded to a team led by Professor Maiken Nedergaard, University of Rochester. The goal of this 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

This MURI began in FY19 and was awarded to a team led by Professor 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; and (2) develop novel experimental systems to challenge and extend the theory and 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 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 nonequilibrium characteristics cause these systems to evolve toward the desired emergent behavior, and (3) design efficient collective computational systems to achieve specific task-oriented goals.

Networked Palynology Models of Pollen and Human Systems

This MURI began in FY19 and was awarded to a team led by Professor 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 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 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 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 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**

This MURI began in FY19 and was awarded to a team led by Professor Sangi Reddy, University of Michigan. The goal of this MURI topic is to determine the mechanisms responsible for radiative heat transfer between the surfaces of nanomaterials and between metasurfaces separated by nanoscale 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 eNFRHT in nanogaps.

One novel and very exciting concept proposed by the team includes a persistent thermal current akin to the quantum Hall effect (QHE). 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.

**Investigating Energy Efficiency, Information Processing, and Control Architectures of Microbial Community Interaction Networks**

This MURI began in FY19 and was awarded to a team led by Professor 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 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, and (4) information exchange between multiple layers of biological organization and the scaling of communication architectures for unicellular organisms to networks of multicellular organisms.
Predicting and Controlling the Response of Particulate Systems through Grain-Scale Engineering

This MURI began in FY19 and was awarded to a team led by Professor José 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, meso, and 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 knowledge across disciplinary boundaries that, historically, have been silos of 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 among theoretical, experimental, and computational approaches covering more than 6 orders of magnitude.

Quantum State Control of Molecular Collision Dynamics

This MURI began in FY19 and was awarded to a team led by Professor 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 study their reactive and nonreactive 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 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 MURI began in FY19 and was awarded to a team led by Professor Ali Jadbabaie-Moghadam, MIT. 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 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, and 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 a DeGroot-style reasoning (a nonlinear, non-Bayesian) system as Bayesian reasoning under certain resource constraints. The proposed work will make use of ideas from nonlinear 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) executing 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**

This MURI began in FY18 and was awarded to a team led by Professor Dirk Englund, MIT. 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 properties 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 include 3D wide bandgap semiconductors (e.g., silicon carbide [SiC], zinc oxide [ZnO], etc.) and recently discovered atomically thin 2D vdW materials (e.g., hexagonal boron nitride [h-BN], WSe$_2$). 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, nonlinear 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 reconstructing 3D and 2D materials fully at the atomic scale, and developing 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 super-radiance/sub-radiance control.

**Multiscale Integration of Neural, Social, and Network Theory to Understand and Predict Transitions from Illness to Wellness**

This MURI began in FY18 and was awarded to a team led by Professor Emily Falk, 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.
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 post-traumatic stress disorder (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**

This MURI began in FY18 and was awarded to a team led by Professor Mingyan Liu, University of Michigan. The goal of this MURI is to create a new compositional game theory framework for characterizing the 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 two-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 that 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 a 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 multiscale framework in which both the coarse-grained model (e.g., of the host population) and the fine-grained model (of the social network of adversaries) need to be reasoned about.

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 plays a role in distributed strategies. The research is addressing inference and decision/control problems. The inference problems involve studies to identify a multiscale 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 MURI began in FY18 and was awarded to a team led by Professor Uwe Kortshagen, 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 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 centimeters 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 demonstrating new material design paradigms on test-bed photonic materials.

Quantum Control Based on Real-Time Environment Analysis by Spectator Qubits

This MURI began in FY18 and was awarded to a team led by Professor Kenneth Brown, 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 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 the 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, ML, 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, ML, 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 are 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.
Science of Embodied Innovation, Learning and Control

This MURI began in FY18 and was awarded to a team led by Professor Daniel Koditschek, 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 among 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; creating new solutions to sensorimotor limitations and challenges represents the second focus.

Stimuli-Responsive Control of Protein-Based Molecular Structure

This MURI began in FY18 and was awarded to a team led by Professor Milan Mrksich, 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.
Toward a Multiscale Theory on Coupled Human Mobility and Environmental Change

This MURI began in FY18 and was awarded to a team led by Professor Rachata Muneepeerakul, University of Florida. 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.

Large-scale environmental changes such as floods, earthquakes, and droughts can drive social mobility, which often precipitate 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 MURI began in FY17 and was awarded to a team led by Professor Andrea Young, University of California, Santa Barbara. The goal of this MURI is to unambiguously realize new systems exhibiting the physics of anyons and 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 2D electronic system. However, the fragility of the FQHE states, in which interesting anyons can exist, has 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

This MURI began in FY17 and was awarded to a team led by Professor Anna Balazs, 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.

Data-Driven Operator Theoretic Schemes to Prediction, Inference, and Control of Systems

This MURI began in FY17 and was awarded to a team led by Professor Igor Mezić, University of California, Santa Barbara. The objective of this MURI is to develop a 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, ML 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; and (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 use of ML algorithms in spectral expansion theory; and (5) use of spectral expansion theory for development of next-generation, real-time computational tools for complex physics with 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, and (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 MURI began in FY17 and was awarded to a team led by Professor Elaine Hsiao, 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, respond to environmental factors (e.g., diet and stress) in a way that modulates host brain activity and behavior. 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 and 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.

**Realizing Cyber Inception: Toward a Science of Personalized Deception for Cyber Defense**

This MURI began in FY17 and was awarded to a team led by Professor Milind Tambe, 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 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. 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.

**Room-Temperature Exciton-Polaritonics**

The MURI began in FY17 and was awarded to a team led by Professor Hui Deng, University of Michigan. The goal of this effort is to explore the use of 2D materials for exciton-polariton systems. Such materials have large exciton binding energies that indicate room-temperature operation may be possible.

Research on 2D materials known as transition metal dichalcogenides (TMDs) has progressed to a degree where the development of Bose–Einstein condensates of exciton-polaritons, which form a coherent light–matter interactive state, is feasible. Such condensates have been shown to emit coherent radiation, equivalent to a laser, at much lower carrier densities than typical photon lasers. Integrated photonics platforms that utilize coherent light could benefit from such room-temperature light sources. The transport of the condensates themselves could also effectively lead to a form of superconductivity for the charged carriers due to the dissipationless propagation of the photonic part of the exciton-polariton. Therefore, exciton-polariton platforms could carry out a number of functions found on photonic circuit platforms but operate at low energies. Important applications for the polariton regimes include short-distance optical interconnects, neuromorphic information processing and computing, and ultra-low energy sensing.

One of the key objectives of Professor Deng’s effort is to explore 2D material science improvements. Specifically, increasing the grain size and production of transferrable 2D nanosheets for integration with microcavities. Another objective of this effort focuses on understanding the stacking behavior of the 2D materials to create nanostructures and interlayer excitons for ultra-low energy effects.
related to switching and polariton control. The research team will also focus on understanding how organic materials determine hybrid TMD-organic polariton effects. The team will pursue these goals by combining state-of-the-art fabrication capabilities with strong experimental and theoretical expertise on polariton physics, 2D materials, photonic devices, and many-body physics in photonic and electronic systems.

**Semantic Information Pursuit for Multimodal Data Analysis**

This MURI began in FY17 and was awarded to a team led by Professor Rene Vidal, 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 multimodal 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 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 MURIS THAT BEGAN IN FY16**

**Closed-Loop Multisensory Brain-Computer Interface for Enhanced Decision Accuracy**

This MURI began in FY16 and was awarded to a team led by Professor Maryam Shanechi, 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 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) ML 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 prototype a BCI for enhanced decision accuracy. The modeling efforts will span Bayesian inference, stochastic control, adaptive signal processing, and ML 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

This MURI began in FY16 and was awarded to a team led by Professor Scott Grafton, 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 noninvasive 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 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 MURI began in FY16 and was awarded to a team led by Professor David Hsieh, 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 that non-adiabatically induces a phase distinct from that existing elsewhere on the ground-state phase diagram. Examples include a nonequilibrium 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 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 nonequilibrium 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 MURI began in FY16 and was awarded to a team led by Professor Christopher Monroe, 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 QIP 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 multidisciplinary 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 QIP 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 QIP 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.

Multimodal Energy Flow at Atomically Engineered Interfaces

This MURI began in FY16 and was awarded to a team led by Professor Donald Brenner, 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 nonequilibrium phenomena 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.

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-nonequilibrium excitations within nanoscale geometries, observe in situ picosecond to microsecond property responses using newly developed methods, inform new theoretical models, and 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 predict their performance.

Sequence-Defined Synthetic Polymers Enabled by Engineered Translation Machinery

This MURI began in FY16 and was awarded to a team led by Professor Michael Jewett, Northwestern University. The goal of this MURI is to engineer the translation machinery to accept and polymerize non-biological monomers in a sequence-defined manner using nontraditional chain growth polycondensation chemistries (beyond amide and ester linkages).

Employing only 4 nucleotides and 20 amino acids, a plethora of biopolymers (e.g., proteins, DNA) with a 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.
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

This MURI began in FY16 and is led by Professor Kang Wang, University of California, Los Angeles. The team consists of researchers from the University of California, Irvine, California Institute of Technology, University of Nebraska, North Carolina State University, and University of Texas at 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 TMDs, and ferromagnetic (FM)/ferri-magnetic/antiferromagnetic (AFM) 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-valleytronics, 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 multifunctional 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.

### Socio-Cultural Attitudinal Networks

This MURI began in FY16 and was awarded to a team led by Professor Larry Davis, University of Maryland (initially led by Professor V. S. Subrahmanian). The goal of this MURI is twofold: (1) develop social science theories to understand latent communication among a small group of adversaries engaged in an effort to deceive and (2) develop multimedia 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 are not only to drive the development of new social science theories, but also drive algorithmic advances in reasoning about joint probability distributions that arise from modeling uncertainties in human actions, speech, gestures, and intentions.
ACTIVE MURIS THAT BEGAN IN FY15

Advanced 2D Organic Networks

This MURI began in FY15 and was granted to a team led by Professor William Dichtel, 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 TMDs.

Emulating the Principles of Impulsive Biological Force Generation

This MURI began in FY15 and was awarded to a team led by Professor Sheila Patek, 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.

Engineering Exotic States of Light with Superconducting Circuits

This MURI began in FY15 and was awarded to a team led by Professor Andrew Houck, 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 nonequilibrium 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, and 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 hundreds of 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 nonequilibrium 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 MURI began in FY15 and is awarded to a team led by Professor George Karniadakis, 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**

This MURI began in FY15 and was awarded to a team led by Professor Ronald Walsworth, Harvard University. The goal of this MURI is to further develop N-V nanodiamonds as non-biological quantum sensors and engineer a biological interface for actuating biological processes.

The N-V center lattice defect in diamond nanoparticles (N-V-diamond) can retain activity in biological environments. Current applications of N-V-diamond include quantum computing, nanoscale magnetometry, super-resolution imaging, and atomic-scale magnetic resonance imaging. These state-of-the-art applications involve N-V-diamonds implanted in substrates; however, recent breakthroughs have allowed isolated nanodiamond 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 N-V-diamond sensitivity, including in the emerging biosensing applications, is that the spectral shape and intensity of optical signals from N-V-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 N-V-diamond’s extreme sensitivity and localization now provide new research opportunities for transitioning N-V-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’s four closely coupled aims are to (1) optimize N-V-nanodiamond synthesis, (2) realize stable, biocompatible nanodiamond surface functionalizations, (3) advance N-V sensitivity to chemical and biological systems, and (4) enable N-V-based manipulation of biological transduction. Systematically studying the integration of N-V 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 AI systems, early diagnosis and effective treatment of neurological disorders at the cellular level, novel human–machine interfaces, and antidotes to neurotoxins and pathogens.

Multiscale Responses in Organized Assemblies

This MURI began in FY15 and was awarded to a team led by Professor Sankaran Thayumanavan, University of Massachusetts Amherst. The goal of this MURI is understanding 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 multiscale 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 multiscale 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 multiscale 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 nonequilibrium 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

This MURI began in FY15 and was awarded to Professor Ambuj Singh, University of California, Santa Barbara, with participation from researchers at the University of Southern California, University of Illinois 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, develop rigorous models that relate interaction patterns and network evolution to task performance, break new ground in the learning of optimal design of teams for complex tasks, and 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.

Noncommutativity in Interdependent Multimodal Data Analysis

This MURI began in FY15 and was awarded to a team led by Professor Rayadurgam Srikant, University of Illinois 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 ML. 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) crowdsourcing in a network of brain–machine interfaces. The framework will provide answers to questions such as the following: What are the fundamental performance limits for noncommutative information collection and processing 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 BCIs will provide new capabilities, including improved time-sensitive, dynamic, multi-source information processing, actuation, and performance prediction guarantees.
ACTIVE MURIS THAT BEGAN IN FY14

Force-Activated Synthetic Biology

This MURI began in FY14 and was awarded to a team led by Professor Margaret Gardel, 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. 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 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, reproduce and analyze these force-activated phenomena in synthetic and virtual materials, and 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 biomimetic material systems.

Innovation in Prokaryotic Evolution

This MURI began in FY14 and was awarded to a team led by Professor Michael Lynch, 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.

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 models that 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; and 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 MURI began in FY14 and was awarded to a team led by Professor Mitchell Luskin, University of Minnesota. This research is co-managed by the Mathematical Sciences and Materials Science Branches. The objective of this project is to develop efficient and reliable multiscale methods to couple atomistic scales to the mesoscopic and 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 (TMDs). 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 by specifically pursuing the following: (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 the 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 vdW heterostructures, will be developed that can reach the timescales necessary for synthesis and processing by chemical vapor deposition and molecular beam epitaxy; and (4) the simulations will be linked to macro and EM modeling 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 biomaterials that are of interest to the Army.

**Multistep Catalysis**

This MURI began in FY14 and was awarded to a team led by Professor Shelley Minteer, University of Utah. The goal of this MURI is to enable multistep 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 multistep 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 multistep 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 multistep 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.

**ACTIVE MURIS THAT BEGAN IN FY13**

**Artificial Cells for a Novel Synthetic Biology Chassis**

This MURI began in FY13 and was awarded to a team led by Professor Neal Devaraj, 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 a chassis for the engineered biological systems and devices. While single-celled organisms are typically used as a 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 that 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).
Appendix

FY21 Broad Agency Announcement
(Online Only)

The chief Broad Agency Announcement (BAA) used by ARO to complete its mission is often referred to as the ARO Core BAA. The ARO Core BAA is open for submissions at any time throughout the year.

The publicly available ARO Core BAA as of the final day of FY20 was W911NF-17-S-0002-07 (i.e., Modification 7 of the FY17-FY22 BAA with eligible submission dates of 1 April 2017–31 March 2022).

This chapter provides key excerpts of the ARO Core BAA: Section II-A (Program Descriptions), which details the research interests of ARO Programs in FY21.

This background image is from “Extreme Polariton Nonlinearity for Next-Generation Computing” on page 45.