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Dynamic Materials, Intelligence, and Power for Future Army Capabilities: A Report of the FY19 Army Science Planning and Strategy Meetings

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1. Introduction

Author: Alexander Kott

This report summarizes the findings of an annual series of meetings. The intent of these meetings is to explore novel scientific opportunities that may lead to providing the US Army with an advantage in future conflicts. The temporal scope of these explorations is strategic in nature, with the time horizon being about 20 to 30 years. The meetings focus on identifying research gaps and barriers that may hinder the achievement of potential novel capabilities, and of possible approaches to overcoming these gaps and barriers. These meetings are called the Army Science Planning and Strategy Meetings (ASPSMs). Numerous research efforts—in-house, collaborative, and extramural—have been initiated or revectorized based on the insights developed during the ASPSMs. This report covers the findings and recommendations developed during four meetings held in the first half of FY19.

1.1 Motivations

Each meeting was motivated by science-informed visions of opportunities and needs of the future battlefield, 20–30 years from now. In particular, in future peer-contested multidomain operations, Army units will be expected to operate at high operational tempos and in decentralized, dispersed fashions, requiring them to be highly mobile and adaptable to the changing battlefield. Operations are becoming increasingly digital and network-centric, with new generations of sensing, weaponry, targeting, fire control, communications, and the integration of robotic and autonomous systems across all echelons. All of these are expected to significantly add to the energy demand of tactical units. An intriguing and emerging way to feasibly exceed the chemical limit is to utilize atomic nuclei as the energy-storage medium. Isomer power sources provide an alternative potential means by which to access nuclear-scale energy storage without relying on fissionable materials. This motivated the meeting titled “Isomer Power Sources”, the subject of Section 2 of this report.

Even if power becomes abundantly available for the future robotics autonomous systems, currently these have operational shortcomings in terms of multifunctionality, the ability to repair and reconstitute on demand, and the capability to conduct armed reconnaissance in areas in which humans and/or biological predators can be highly effective. To disrupt this paradigm, the generation beyond the next generation of robotics and autonomous systems will need to combine levels of mechanical work, adaptation, repair, energy efficiency, and information processing that are reminiscent of biological organisms. An

underlying feature of biological systems that supports these functionalities is that of nonequilibrium materials with emergent macroscopic properties. New scientific opportunities seem to be emerging at the intersection of stimuli-responsive materials, mechanical metamaterials, distributed chemical control, and our ability to “program” macroscopic properties and dynamic response. These thoughts underpinned the meeting titled “Chemostructural Dynamics” (Section 3).

As materials (and their manufacture) become increasingly more complex, the investments in materials and manufacturing research over recent decades have trended to increasing emphasis on modeling to drive understanding and improve experimentation efficiency. Despite advances in computational capabilities, we are still far from capturing relevant chemistry and physics where there is significant complexity. In addition, additive manufacturing leads to capability for mixing materials and modulating material properties almost arbitrarily within a monolithic component. This significant reduction in design constraints is extremely powerful in terms of producing components with extraordinary performance, but optimal solutions (especially for multiphysics applications) may be highly nonintuitive and complex to identify or define. To accelerate the pace of technology development to deliver new capabilities to the warfighter, the Army must accept and address the key bottleneck limiting the adoption of advanced technologies: the complexity of design. This inspired the meeting titled “Materials Data and Design Science for Materiel on Demand and by Design” (Section 4).

Furthermore, future Army intelligent systems are expected to learn from a variety of experiences; interact with autonomous agents, soldiers, and experts; and use and update stored shared information. These systems will require long-term memory that can be updated in real time, queried for inference and reasoning, and support Soldier–system interaction and semantic dialog. Opportunities are emerging to combine autonomous control, real-time learning, and memory in the form of knowledge bases (KBs). These require bringing together experts in robotics and autonomy, deep learning for perception, semantic reasoning, and KB construction and querying. Currently, the autonomy and semantic KB research communities are largely separate. To draw from both areas, consider the cross-disciplinary intelligent systems issues, and identify key research questions and collaborative multidisciplinary research areas were key goals of the meeting titled “Real-Time Learning, Knowledge Bases, and Information Retrieval” (Section 5).

1.2 Key Findings

The meeting titled “Isomer Power Sources” found, inter alia, the following:

- The effect called nuclear excitation by electron capture, NEEC, may prove to be a practical way to utilize isomers for future Army energy and power sources on the battlefield. In particular, the ASPSM participants concurred that isomer-based approaches have the potential to be used as a method to drive heat engines for extreme duration autonomous system operation. It was also acknowledged that while the concept has disruptive potential, the research in this area is at a very early stage. A consensus course of action was that the primary research goals at the present time, in order to move the technology toward this vision, must be to confirm that NEEC can occur for other isomers, whether or not they are suitable for future applications, and to fully characterize how the effect works. This would include determination of an excitation function.
- The participants also recommended that a system-level integration study should be conducted to guide the optimal design of a heat engine for a given propulsion system. Stirling engines developed for combined heat and power, space applications, and solar energy conversion have very different requirements than one developed for a propulsion system.
- A key area identified for needed future investment in order to realize an integrated isomer power source was the exploration of thermal energy storage (TES) materials that exploit the latent heat of fusion (e.g., molten silicon) for providing load leveling at the cost of extra mass. The R&D will also need to characterize the lifetime of the system, which would require experiments to cycle devices up to thousands of cycles.

The meeting titled “Chemostructural Dynamics” recommended the following priorities for future research:

- Develop principles of chemostructural inverse design: How do we translate macroscopic goals into reversible, embedded chemical reactivity, design of active subunits, topological order, and so on?
- Develop efficient control approaches leveraging combinations of active and passive units as a more efficient construct than fully active.
- Determine the energetic costs of maintaining a state of nonequilibrium and how this translates to useful macroscopic functionality, properties, and constitutive law behaviors.

- Explore how biology can play a role beyond serving as a motivational template. Can biohybrid constructs be assembled, stabilized, and efficiently controlled?
- Develop methods to focus the energy of a mechanical wave so as to produce a measurable electrical signal through an ion reaction material.
- Develop first principles from the union of mechanochemistry, elasticity, and thermodynamics for a new field of active matter for chemomechanical systems.

The meeting titled “Materials Data and Design Science for Materiel on Demand and by Design” yielded a number of findings and recommendations:

- Advancements in the capability to design, synthesize, and process compositionally complex materials are not being matched by advancements in materiel design tools which can incorporate that scalable complexity into components and systems. There is a unique opportunity to significantly advance materiel performance by taking advantage of material inhomogeneity and ultimately driving material modulation as a design parameter by investing in the science of design.
 - Recommendation: Support a collaborative research effort among Army, academia, and industry to develop modular design tools with point-wise material property design freedom enabling material inhomogeneity down to the smallest scales.
- New materials systems and manufacturing technologies, and their associated models, are not coordinated to enable the construction of high-performance design workflows. An integrative knowledge construct would enable Army to more rapidly transition technology and field the most advanced materiel, adapt and adjust to emerging threats and conditions, and efficiently assimilate new technologies developed elsewhere. Because such a framework would necessitate open standards for models and data, the inputs would serve as persistent and actionable embodiments of research knowledge products.
 - Recommendation: Support a tri-service and cross-governmental coordinated program to form an open design framework with adequate scale to attract academic and industrial participation. A critical piece of this framework is development of a shared multiscale design software language to efficiently describe constraining requirements and optimize performance.

- Current objective functions are limited to design parameters with clear mathematical representation and implementation in a static design cycle, limiting the range and agility of materiel design through manufacturing.
 - Recommendation: Support internal and extramural efforts to develop “soft” objective functions, such as those involving human response, and real-time objective functions enabling dynamic design and agile threat-responsive manufacturing that can readily incorporate recent innovations into any stage of the design cycle.

The key findings of the “Real-Time Learning, Knowledge Bases, and Information Retrieval” meeting include the following:

- Dramatic but separate progress over the past decade has occurred in Artificial Intelligence (AI) for autonomous control and robotics, as well as semantic processing and KBs. While these two research communities are largely distinct, there is a significant opportunity to create a new multidisciplinary approach to Army intelligent systems that has high payoff.
- Current work on semantic simultaneous localization and tracking (semantic-SLAM) is an early step in this direction, combining traditional robotic-sensor-based SLAM with semantic information about the scene, such as object labels. Envisioned more broadly, the ability to link and apply reasoning among geometry, mapping, and objects in the scene will lead to leap-ahead cognitive capability.
- Research should focus on developing human–KB querying methods and linking these with human–autonomy (human–agent teaming) research. Such research includes machine–KB interaction and graph-based and other formalisms to provide unifying analytical frameworks that lead to mathematical bridges between autonomy and KBs.

2. Isomer Power Sources

Authors: James J Carroll, Christopher J Chiara, Justin L Shumaker, and Brett H Piekarski

2.1 Vision

In future peer-contested multidomain operations, Army units will be required to operate at high operational tempos and in decentralized, dispersed, and semi-independent fashions, requiring them to be highly mobile and adaptable to the changing battlefield. The battlefield of the future is also expected to become increasingly digital and network-centric, with new generations of sensing, weaponry, targeting, fire control, communications, and the integration of robotic and autonomous systems across all echelons. All of these are expected to significantly add to the energy demand of tactical units. This increase has not been matched by innovations in the ability to generate power, convert and store energy, or manage and distribute power. Achieving these dispersed and potentially longer-duration maneuver missions, with limited opportunity for resupply, will require innovative solutions for more energy-dense and efficient energy sources. This was recently recognized outside DoD by the US Department of Energy in a statement that “the DoD needs all available power all the time.”¹ While considerable effort is being expended at improving energy storage and delivery in many forms, it is also clear that the use of chemicals, such as logistics fuels, as the foundation of Army energy presents a fundamental constraint—a “chemical limit”²—on available energy density. An intriguing and emerging way to feasibly exceed the chemical limit is to utilize atomic nuclei as the energy-storage medium. For the nearer term, concepts for the use of “compact”, “modular”, or “micro” nuclear (fission) reactors are being explored to power medium to large bases, as apparent in the DoD Strategic Capabilities Office Request for Information RFI-01182019-RD-WHS019.* However, even if realized as envisioned, such fission reactors are not suitable for Soldier or autonomous platform power on the tactical edge, as they are simply too large to be transported effectively on a flexible basis.

Isomer power sources provide an alternative potential means by which to access nuclear-scale energy storage without relying on fissionable materials. Isomeric materials contain about 100,000 times the intrinsic energy density of chemical fuels, in turn far greater than that of chemical batteries, which suggests much lower fuel weight for a given power requirement. Of even larger practical impact is the

* RFI small mobile nuclear reactor. Government Contracts; 2019 Jan 22 [accessed 2019 July 3]. <https://www.governmentcontracts.us/government-contracts/opportunity-details/NBD00159828114221413.htm?cts=148f0>

potential to enable greatly extended mission durations. For example, an autonomous 5-HP Squad Mission Equipment Transport (SMET) vehicle equipped with an efficient diesel engine might achieve 2–3 days of endurance with greater than 100 kg of fuel while the same vehicle powered from an isomer heat engine could operate continuously for more than half a year with less than 1 kg of ^{242}Am . Such capabilities would represent a truly disruptive advance in energy and power for Army applications. However, considerable basic research will be required before the feasibility of such an advance can be assessed.

2.2 Objective and Scope

This ASPSM sought to identify scientific plans and challenges for basic research to characterize a particular new process for controlling an energy release from isomeric materials and to determine if that process can be used for a practical and novel heat source. The meeting also sought to identify the critical steps and directions for research to develop effective and scalable approaches toward the conversion of heat from such a novel power source into useful electrical power for applications such as the propulsion of future autonomous vehicles. Numerous fundamental questions exist for the new process, so it is quite early to begin examining practical aspects of an isomer power source. However, it was determined to be beneficial to bring together both nuclear physicists and heat conversion subject matter experts to initiate an interface between basic research, applied research, and developmental engineering aspects at this early stage. Doing so would help inform both research communities as to the challenges and critical issues from both perspectives. To accomplish this, two subtopic areas were organized, and participants were selected for their expertise and abilities to contribute in these areas:

- 1) *Characterization and understanding of NEEC for an isomer power source:* This area considers the state-of-the-art in experimental techniques and how those techniques could be used to answer fundamental questions on the newly discovered process called NEEC (nuclear excitation by electron capture), which would be the basis for controlled energy release of energy from isomeric materials.
- 2) *Energy conversion and utilization from an isomer power source:* This area considers all practical methods and technologies to efficiently convert heat energy into electrical and/or mechanical work for use in a ground propulsion system.

2.3 Background

Radioisotopes are unstable atomic nuclei that decay with a characteristic time scale, or half-life. This decay results in transmutation of the nuclide into another nuclide, with an accompanying release of energy in the form of the emission of charged particles and photons. Prior to the decay, the energy is stored in the binding energy of the constituent nucleons (i.e., neutrons and protons) and is on the order of 100,000 times greater per unit mass than even the theoretically most-energetic chemical. The reason is simple: Bonds between nucleons are 100,000 times stronger than those between atoms or molecules. Thus, radioisotopes have been referred to as “ultra-energy materials” and could provide a way to access energy storage beyond the “chemical limit”.² Perhaps more importantly, radioisotopes with long half-lives (e.g., tritium (^3H) with a half-life of 12.7 years) retain their energy effectively and could provide durable energy for a variety of applications like drop-and-forget sensors.³

The durable energy of long-lived radioisotopes, however, is coupled with a lower power level, as the released power per unit mass is proportional to the reciprocal of the half-life: Longer half-life means lower intrinsic power density. Thus, to achieve large power output, as required for a platform, would necessitate a relatively large amount of radioisotope “fuel”. The alternative would be to use a smaller amount of a shorter-lived radioisotope, but then the radioisotope may not even last long enough after its production to reach a point of use. A way to bridge this power gap for radioisotopes may be to use an exotic type called a nuclear isomer.

The nucleons within atomic nuclei are a dynamic system that can exist in many states of differing energies, half-lives, and other measureable properties. For example, more than 100 excited states have been observed for the nuclide ^{180}Ta .⁴ When the properties are quite different between a specific state and those at lower energies to which it could decay (by emitting a gamma ray, leaving it as the same nuclide), that state can have a long half-life. This occurs for ^{180}Ta , where an excited state storing 77 keV (i.e., 41 MJ/g) has a half-life that measurements show is *at least* 2×10^{16} years. Such a metastable nuclear excited state is called a nuclear isomer.⁵ Amazingly, the lowest-energy state of ^{180}Ta (the ground state) has a half-life of only 8.2 h and decays by β^- (electron) emission to release further energy. Thus, one could conceive of collecting ^{180}Ta in the isomer state for energy storage (straightforward, since it occurs naturally in the isomer), sitting that material on a shelf until the energy was needed, then transforming those nuclei from the isomer into the higher-power, energy-releasing ground state. This would then be a switchable radioisotope for a power supply.

This type of transformation has been experimentally demonstrated for ^{180}Ta , best characterized in the work of Belic et al.,⁶ although the energy input required to switch from isomer to ground state was too large to serve in a practical application. As of today, five other isomers of different nuclides have been switched (“depleted” is the more typical scientific term). For example, the nuclide ^{108}Ag has an isomer with a half-life for energy storage of 438 years. It was demonstrated in 2012⁷ that the isomer could be transformed to the corresponding ground state having a half-life of 2.4 min using x-rays. Further characterization of the switching (or depletion) processes is underway for many of the 11 known isomers with half-lives greater than 1 year, convenient for energy storage.² So far, mechanisms for switching exist, but most appear to be of low efficiency for causing the needed transformation.

A new mechanism for isomer switching was recently discovered and published in the prestigious journal *Nature* in February 2018.⁸ This mechanism relied on an effect first proposed in 1976, but never before observed, in which manipulation of atomic electrons could excite the corresponding atomic nucleus. The key point is that the atom is 100,000 times larger than the nucleus. The probability for causing an energy release from an isomer by interaction with the atomic electrons should be much higher than other mechanisms that require a direct interaction on our part with the nucleus. The effect is called nuclear excitation by electron capture (NEEC) and may prove to be a practical way to utilize isomers for Army energy and power.

The initial demonstration of NEEC was performed using a nuclide optimized for that test, but not optimal for energy storage. Additional cutting-edge research must fully characterize the process and then determine if it can be adapted to a more energy-favorable isomer like ^{242}Am . This nuclide has an isomer with a half-life of 141 years, convenient for production and storage of the material. Once switched to the ground state, the resulting decays proceed first with a 16-h half-life, followed by a 163-day half-life, both primarily by charged-particle emission. The decay radiation is relatively easily captured to produce heat, comprising an attractive and novel nuclear-scale power source of very long duration (only a 6% loss of power output every 2 weeks after the 16-h phase is complete).

It is already possible to consider the advantages of this material. If ^{242}Am is used, for example, the total intrinsic energy density of the material in solid form is about 3% that of uranium (and about 60,000 times the energy density of JP-8). Assuming 10% efficiency for the process of isomer depletion and subsequent energy harvesting, a 5-HP anticipated need for operation of a SMET ground vehicle, the mass of material scales with the power for missions of the same duration (i.e., less than 1 kg of ^{242}Am would be needed for 163 days of continuous operation). For shorter missions, however, less material (compared to the amount scaled by time)

would be needed because the power level is higher initially (since there is higher power output during the 16-h decay period and the start of the 163-day period).

The main practical aspects to be resolved in order to utilize an isomer power (heat) source for DoD applications are 1) the scale of the switching apparatus—for example, building- or truck-sized equipment, mobile (near the point of use) or stationary (far from the point of use, requiring transport of switched material); 2) the availability, production, and purification of energy-relevant isomer materials; and 3) the optimal heat-to-useful-energy conversion and storage methods for different applications. For the third aspect, a variety of thermal management and conversion technologies are available and under consideration, including the use of solid-state devices such as thermoelectric and thermophotovoltaic for direct production of electricity (e.g., an adaptation of NASA-style radioisotope thermoelectric generators [RTGs]). The use of Stirling cycle and other heat engine variants presently offers the highest conversion efficiency for heat-to-electricity. All of these heat conversion technologies, in the context of propulsion systems, are not yet in widespread use and would benefit substantially from additional R&D in order to reach their theoretical limits for both efficiency and power density at the scales appropriate for medium to small unmanned ground vehicles and unmanned aircraft systems. CCDC Army Research Laboratory's (CCDC ARL's) Sensors and Electron Devices and Vehicle Technology Directorates are involved in this work. The first aspect is sensitively dependent upon the particular details of the newly discovered switching process; for example, does it require an implantation-style approach (as used in the original demonstration—isomers implanted into a solid material) or could a stationary isomer target be exposed to a beam of electrons? In either case, the scale of the apparatus will depend on the energy required for the production of appropriate conditions for switching.

2.4 Challenges, Key Research Questions, and Recommendations

The ASPSM on Isomer Power Sources was organized to facilitate cross-disciplinary discussions between participants with expertise matched to the two subtopic areas, while also enabling in-depth consideration of specific challenges within each of those areas. Each breakout group discussion addressed:

- Overall vision for future; impact to Army systems
- Scientific challenges and open underlying science questions
- Innovative solutions and scientific plans to address challenges
- Systems view and interdependencies between power sources and energy conversion technologies

The following summarizes the outcome of those discussions.

Topic Area 1: Characterization and understanding of NEEC for an isomer power source.

Key Discussion Points and Research Questions:

- As an example of entirely new physics, never before observed experimentally, the central question is, How does NEEC work? The general concept was introduced many decades ago⁹ and was proposed in 2002¹⁰ as a possible means of isomer switching (typically called “depletion” in the nuclear physics literature). However, a detailed understanding of how NEEC functions in a real situation is not yet available.
- Since the NEEC effect was only demonstrated recently for the first time, there have been no prior measured results with which to test the validity of theoretical models. In addition, no detailed theoretical calculations were previously attempted for the particular approach used in the NEEC demonstration experiment.
- The initial observation of NEEC was obtained using an implantation-style (“beam-based”) scenario. If NEEC can only be produced in this scenario, it is likely that a practical application would require a long-lived isomer to be switched at a moderate- or large-scale facility and then transported to the point of use. If NEEC or other depletion mechanisms could be produced in a reversed scenario, where photons or electrons could be injected into stationary isomer materials, then it might be possible to use smaller-scale switching devices near or at the point of use.
- As emphasized by Dracoulis, “Every nucleus is unique.”¹¹ This means that even when the NEEC process is fully characterized, there will be differences in its application based on the specific properties of each isomer (of different nuclides). It also means that experiments on different nuclides will likely require specialized techniques unique to each nuclide.
- The atomic nucleus, for moderate to large atomic mass, is a complex N-body system of interacting nucleons (neutrons and protons). The current state-of-the-art in computing cannot exactly solve problems involving $N > 2$ interacting bodies, yet the nuclides of greatest interest for isomer power have $N > 30$. Also, a complete formulation of the two-body nuclear strong force is still lacking, which is another impediment to accurate nuclear models. It is possible that quantum computing may be useful in the future for these calculations. Ultimately, it is not possible at present to accurately

calculate the rates for transitions between nuclear states participating in the NEEC process.

- A variation on NEEC, using muon capture instead of electron capture, may be possible and might lead to larger cross sections (greater efficiency) for switching. This process has never been examined theoretically or experimentally. Even if the cross section was larger, difficulties in producing muons for capture may preclude this idea.
- There was considerable detailed discussion of various experimental techniques and facilities that could be used to better understand NEEC and isomer depletion.
- There was some discussion of historical false steps in isomer research by previous researchers that were based on unconfirmed results, yet oversold prematurely for programs.

Recommendations for Future Research and Investment:

- The primary research goals at the present time must be to confirm that NEEC can occur for other isomers, whether or not they are suitable for future applications, and to fully characterize how the effect works. This would include determining an excitation function, giving the probability of the NEEC process as a function of the energy used in the experimental scenario. A 5-year period is a reasonable expectation for this research but could be shorter or longer as unforeseen difficulties could arise.
- A low-energy Coulomb excitation experiment could be performed by which to estimate the $B(E2)$ strength of the potential NEEC transition for switching ^{242}Am .
- While NEEC as a switching mechanism and ^{242}Am appear the most attractive prospects at the present time, other mechanisms such as super-elastic neutron scattering and other long-lived isomers may prove to be as or more important. Again, research results will determine the practicality of any mechanism and isomer.
- Separate efforts should be made to investigate the feasibility of producing specific isomers in sufficient quantities for tests and eventual prototypes.
- The ARL research effort into NEEC and isomers is at the cutting edge and relies on an extensive network of interested colleagues who join with ARL subject matter experts on an ad hoc basis to study particular aspects of the problem. This expands the expertise that can be brought to bear on isomer research in a very cost-effective way. However, it might be advantageous

to assemble a regularly convened advisory committee of scientists to provide fresh perspectives and ideas, and to help prioritize research thrusts.

- Wherever possible, perform research on parallel tracks (e.g., NEEC tests and isomer production studies). It is clear, however, that many experiments will follow a serial approach as NEEC is investigated.
- ARL should continue to partner with appropriate expertise and specialized facilities domestically and abroad to maintain the pace of research. The ability to utilize an “extended virtual laboratory” is a major advantage to be exploited in this field. At all times, the key is to maintain the present firm foundation of science in this research area: “do good science”, “have good evidence”, “don’t overpromise”.

Topic Area 2: Energy conversion and utilization from an isomer power source.

Key Discussion Points and Research Questions:

- Several energy conversion technologies were represented by experts in the areas of thermophotovoltaics (TPVs), thermoelectrics (TEs), and Stirling cycle engines. Also present were experts in the areas of thermal energy storage, heat exchangers, and RTGs.
- Systems requiring greater than 2-kW electrical power should utilize Stirling cycle engines to achieve the greatest efficiency and power density.
- TE and TPV technologies require additional R&D to reach Stirling engine efficiencies but could compete with Stirling cycle for those systems requiring less than 2 kW.
- The acoustic signature of free-piston Stirling engines is considered a silent technology and pairs of engines are often utilized to cancel mechanical vibration.
- While some Stirling cycle engines may work for aerial fixed-wing applications, the isomer-powered propulsion system is likely to be one that is ground based given the strict power-density requirements needed for aircraft.
- The power obtained from all of the conversion technologies is likely to be electrical given the typical power transients for a ground vehicle.
- The format and operating temperature of the isomer power source are unknown, and therefore the means of developing the optimal heat exchanger for thermal conversion is an open question.

- Without a concept of operations (CONOPs) for a notional mission, it is difficult to develop requirements for the thermal energy conversion system.
- What is the optimal geometry for a heat engine that operates from an isomer heat source? Could the engine be wrapped around the heat source?
- What opportunities exist to improve power density for an application-specific heat engine designed for propulsion?
- Could additive manufacturing for certain components of TPVs and Stirling engines improve efficiency through the design of geometries that were previously impossible to manufacture? One example is the heat exchanger.

Recommendations for Future Research and Investment:

- A system-level integration study should be conducted to guide the optimal design of a heat engine for a given propulsion system. Stirling engines developed for combined heat and power, space applications, and solar energy conversion have very different requirements than one developed for a propulsion system.
- Further R&D is required to develop higher-temperature materials, which will further improve the efficiency of Stirling engines. It is worth noting that SoA free-piston Stirling engines are presently at or above 42% thermal conversion efficiency for small engines having an electrical output between 1 and 2 kW operating between 650 and 850 °C.
- Further R&D is needed in additive manufacturing for Stirling engines and heat exchanger components. Research in this area is new and shows promising results, specifically 3-D-printed Inconel engine components.
 - Greater control over metal grain structure during the printing process is needed to achieve the performance of conventional manufacturing processes (e.g., investment casting and machining).
 - The printing of specialty metals (refractory metals) is needed for both Stirling and TPV components. In the case of TPV, the materials would include tantalum and tungsten.
 - Heat exchanger geometries that provide optimal transfer of heat from an isomer to the hot section of the engine, TPV or TE.
 - The printing of metal heterogeneous/gradient materials for the Stirling regenerator for improved adiabatic efficiency.

- Heat treating of additively manufactured metal components to ensure maximum strength under typical high-temperature and high-pressure operating conditions.
- It is assumed that isomer materials will be the dominant cost. A significant cost of the Stirling cycle heat engine is the high-temperature materials to ensure a mean time between failure (MTBF) on the order of many thousands of hours. An idea to utilize more conventional high-temperature materials (lowering the MTBF) to lower cost yet retain similar efficiencies was presented. Modern free-piston Stirling engines have an MTBF of 80,000 h while the vehicle it operates on is likely to have less than 2,000 h.
- Thermal energy storage materials exploiting latent heat of fusion (e.g., molten silicon) would provide load leveling at the cost of extra mass, but further research to design such a system would be required.
 - The TES system will require R&D to characterize thermal performance to/from system, design to achieve high power and heat flux, convective coupling, and lifetime-involving experiments to cycle devices up to thousands of cycles.
 - An exploration of the microstructure of the heat exchanger to improve performance and effectiveness of thermal energy storage.
- Magnetic materials having greater flux density and/or higher Curie temperature, beyond that of neodymium and samarium cobalt, would reduce the mass of the linear alternators and increase operating temperature. Research in new magnetic materials (e.g., iron nitride) may hold the key.
- ARL Specific:
 - Investment into facilities for testing high-temperature heat exchangers above 900 °C and above 3-kW heat output for materials research and testing. Very few facilities offer these capabilities.
 - Facility to perform destructive and endurance testing for multiple (10+) thermal conversion systems.
 - Hire or support high-temperature materials metallurgist with 3-D printing expertise to look at test articles and contamination.
 - Build a thermal materials program with expertise in thermal energy storage and heat exchangers.
- Lithium battery technology appears to be the best method of transferring energy between vehicles, more so than thermal energy storage.

- The CONOPs for how and when the isomer power source would be utilized should be articulated to develop the requirements to design an appropriate thermal energy conversion system.

2.5 Summary

The development of an isomer power (heat) source could be a disruptive advance in energy and power for Army applications. It could enable greatly extended mission durations while, by tapping into the tremendous intrinsic energy density of atomic nuclei, simultaneously reducing the weight of fuel (or batteries) for Soldier or platform use. The greatest challenges at present lie in the realm of basic research, in that considerable effort must be made to assess the feasibility of switching of isomers from long-lived energy-storing states for accumulation and transportation of isomer materials into shorter-lived (but still long enough for extended missions) energy-releasing states. The recent discovery of a new physical effect, nuclear excitation by electron capture (NEEC), may serve as the basis for such isomer switching (typically called depletion in the literature). Additionally, considerable research and engineering will be necessary once the optimum isomer and switching mechanism are identified to produce efficient heat-to-useful-energy conversion from an isomer power source. While high risk, the potential benefits of an isomer power source are great, and further research is clearly justified and needed to investigate the feasibility of this potentially disruptive technology.

Some key points were raised during the breakout sessions along with recommendations on how the community could move forward in addressing open research questions. A few of the major points raised include the following:

- A detailed understanding of how NEEC functions in a real situation is not yet available and more research is needed to develop and test the validity of theoretical models.
- The NEEC effect was only demonstrated recently for the first time; future efforts need to confirm that NEEC can occur for other isomers.
- Other isomers that are more relevant to Army applications and potentially autonomous vehicle propulsion need to be explored. The production and refinement of these isomers also need to be addressed.
- The infrastructure and scalability of the mechanisms to trigger the NEEC effect will dictate how this approach could eventually be used in practice.

- There are currently only limited experimental techniques and facilities available for this type of research, which could limit the rate of advancement.
- While the NEEC research is still very nascent, a system-level integration study could be beneficial to guide the optimal design of a heat engine for future propulsion systems based on NEEC technology.

The participants were from diverse and international backgrounds. While they agreed the research into isomer power is still at a very early stage with many unknowns, they also agreed that it was beneficial to bring together the basic research, applied research, and engineering development communities together at an early stage. A theme that emerged from the discussion was that efforts should be made to build and strengthen the community around this topic given the number of materials to be explored, the need for increased generation and sharing of data, the need for parallel research tracks, and the potential for leveraging the relevant facilities located within and outside of the United States. Focused growth of the community around this topic is important to realize the potential for achieving an isomer power source.

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3. Chemostructural Dynamics

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The Army has initiated studies of the future battlefield environment beyond 2020 and the expectation that near-peer adversaries will employ autonomous systems and AI to integrate across multiple domains (e.g., “Operationalizing Robotic & Autonomous Systems in Support of Multi-Domain Operations,” 2018 Nov, ARCIC Future Warfare Division). In order to combat a near peer with such capabilities, it is expected that the Army will become increasingly reliant on robotics autonomous systems, which have operational shortcomings in terms of multifunctionality, the ability to repair and reconstitute on-demand, and the capability to conduct armed reconnaissance in areas in which humans and/or biological predators can. In order to disrupt this paradigm, the generation beyond the next generation of robotics and autonomous systems will need to combine levels of mechanical work, adaptation, repair, energy efficiency, and information processing that are reminiscent of biological organisms. An underlying feature of biological systems that supports these functionalities is that of nonequilibrium materials with emergent macroscopic properties. Future adaptive Army systems will leverage advances in new interdisciplinary foundational scientific directions that bring together scientists in chemistry, materials science, active matter physics, elasticity/continuum mechanics, and structural dynamics to explore future directions in nano/micro-architected active matter and structures leveraging distributed, reversible chemical reactivity and responsivity to stimuli for macroscopic functionality.

3.1 Objective and Scope

This ASPSM brought together scientists in chemistry, materials science, active matter physics, elasticity/continuum mechanics, and structural dynamics to explore basic research questions and future directions in nano/micro-architected active matter and structures leveraging distributed, reversible chemical reactivity and responsivity to stimuli for macroscopic functionality. The workshop used a nontraditional, interactive format relying almost entirely on small-group breakout sessions to identify new collaborations and drive discussion. The workshop began with 5-min introductory presentations from the academic scientists to briefly discuss their research interests and capabilities relevant to the topic area. Following the presentations, the participants were organized into small groups and tasked to identify new scientific opportunities at the intersection of stimuli-responsive materials, mechanical metamaterials, distributed chemical control, our ability to “program” macroscopic properties and dynamic response, key barriers to achieving

these opportunities, and strategies for how interdisciplinary groups might interact to succeed in developing a program of research to achieve novel capabilities or generate new scientific domains.

3.2 Background

Classical metamaterials research has demonstrated the potential for micro-architected materials to surpass the intrinsic properties and functionality of natural and conventional materials. Metamaterials now exhibit a range of novel electromagnetic, acoustic, or mechanical phenomena such as negative bulk properties (negative Poisson ratio, compressibility, or refractive index), advanced wave tuning (attenuation, guiding, and cloaking), as well as topological invariances and protection. However, most examples of exceptional functionality stem from subunit architectures exceeding micrometer length scales, fixed lattice topologies, and chemically inert material constituents. Provided that the wealth of remarkable properties manifest within essentially static and passive structures, the opportunity to elicit novel behaviors and properties from dynamic and chemically active metamaterials is compelling. Moreover, the promise of new functionalities derived from advances in precision control of subunit architectures with nanoscale structural complexity opens the door to stimuli-responsive constituents and distributed chemical triggering.

Several recent and pioneering breakthroughs suggest that a new frontier of active metamaterials with precise and dynamically tunable properties is within reach. For example, nanomaterial assembly research has achieved order-of-magnitude advancement from micrometer subunit architectures to nanoscale supramolecular superlattices. Researchers have demonstrated colloidal single-crystal synthesis with 3-D patterns of ordered nanoparticles as well as nanomaterial assembly onto surfaces with systematically controlled 3-D periodicity. The importance of interfacial phases in nanocrystalline materials has led to computational and characterization tools for their study. Additionally, notable advances in distributed chemical triggering mechanisms now enable mechanical property tuning by coupling hierarchical supramolecular assemblies to specified external inputs. Hierarchical supramolecular assembly research has led to artificial muscle-like functionality in materials comprising photomechanical molecular motors (Chen et al, *Nature Chemistry*, 2018) as well as stimuli-responsive polymer matrix “superlattices.” The former has potential to modulate bulk properties from nanoscale sensitivity to thermal, chemical, electrical, optical, or other inputs. Together, these breakthroughs represent significant advances in precise nanoscale structural control, enable fundamentally new forms of matter with unusual and useful properties, and permit fabrication of a wide range of materials.

Moreover, functionality need not be limited to static module architectures. By leveraging dynamics, patterns of activity in mechanochemical oscillators (e.g., Belousov–Zhabotinsky [BZ] oscillators) and mechanochemical reaction networks could seed future materials capable of chemical morphogenesis. Stimuli-responsive unit cells might experience instabilities leading to changes in morphology (emulating embryogenic behaviors). Engineering the particular properties of the instabilities will depend on the “structural” aspects of the unit cells. That is, the finite extent, boundary conditions, mode shapes, and so on, will play a significant role.

However, despite all the recent metamaterial advances and the promising future of nanoscale architectural control, consideration of global structural and load-bearing aspects of such materials domain is almost nonexistent. There is fresh opportunity to challenge communities typically focused on small-scale phenomena to consider the impact from global stress fields, the role of finite extent leading and boundary conditions, mode shapes, buckling morphologies, and so on. How intrinsic functionality and activity might modulate large-scale features is a fairly unexplored domain that would also significantly benefit Army and other DoD-relevant problems facing structural dynamics.

3.3 Gaps and Recommendations

Several observations, technical gaps, and recommendations came out of the ASPSM discussions and breakout sessions. Some general observations were the following:

- Currently, there is insufficient understanding of the underlying thermodynamic and kinetic factors needed to develop the design principles, processes, and precise nanoscale structural control required for fabrication of mechanical metamaterials with responsive functionality. Controlling the architecture of metamaterials down to the nanoscale is challenging but critical for designing materials with the desired functionality.
- Development of quantitative, high-resolution analysis techniques for spatiotemporal characterization and in-situ study of interphase and interfacial behavior at the nanoscale is a high priority.
- There are few fabrication/processing techniques compatible with responsive composite materials.
- Models for the coupling between chemical reactions and elastic–plastic deformations are predominantly phenomenological.

- There has been very little work on studying how to drive electrochemistry with energy transduction materials. Most work is on electrochemistry driven by external power sources.
- Approaches are needed to enable fabrication of heterogeneous materials with integrated energy transducers.
- There is a lack of understanding of how multiple electrochemical reactions interact with each other and develop emergent behavior. How can we leverage computational tools, perhaps machine learning, to do this faster?

Suggested research areas include, but are not limited to, the following:

- Theoretical and computational methodologies capturing essential structure-function-stimuli relationships that enable predictive understanding of targeted nano-architectures and interfacial phase dynamics.
- Experimental synthesis and characterization techniques for dynamic structural control (e.g., stimuli-responsive interparticle separation) as well as tailored phases transformation with consistent and measurable responses to external stimuli.
- Novel precision measurement of desired mechanical properties at the constituent level, at the unit-cell level, or at selected limited locations and interfacial boundaries.
- Control of chemo-mechanical interactions exploiting topological properties for bulk mechanical property changes or interfacial phase transformations.
- Advanced metamaterial-enabled tailoring of the transmission, absorption, filtering, and guiding of waves and mechanical loads (e.g., parity-time symmetry, coherent virtual absorption, nonreciprocity and directional gain, active and tunable topological protection).
- Striking the right balance between complex enough for function, but simple enough for mass manufacturing for scalable materials.
- Engineering macroscopic material form capable of altering the molecular, nano, and microscale ordering, to realize bioinspired hierarchical materials.
- Low temperature, fast, and nondisruptive processing methodologies.
- Beyond BZ chemomechanical oscillators: adopt a paradigm in which the rapid, excitatory part of an oscillatory sequence is in an autocatalytic chemical reaction and the slow, inhibitory part is in the mechanical response.

Some Key Research Questions:

- Inverse design: How do we translate macroscopic goals into reversible, embedded chemical reactivity, design of active subunits, topological order, and so on?
- What are the appropriate metrics to use for the design of structures formed of underlying dynamical systems?
- What are the most efficient control approaches? Can we leverage combinations of active and passive units as a more efficient construct than fully active?
- How do the energetic costs of maintaining a state of nonequilibrium translate into useful macroscopic functionality?
- What is the role of biology beyond serving as motivational templates? Can biohybrid constructs be efficiently controlled?
- How do we focus the energy of a mechanical wave so as to produce a measurable electrical signal through an ion reaction material?
- Can the new field of active matter guide a general modelling framework for chemomechanical systems?

3.4 Conclusions

There are significant opportunities and challenges facing the future of chemomechanical structural materials. However, a long-term fundamental research effort will enable future material systems capable of intrinsic and distributed computation, control, and actuation for applications ranging to novel actuators for robotic systems to smart, reconfigurable composites for vehicle systems. The scientific community is prepared for the challenge but needs the resources to enable the necessary interdisciplinary interactions.

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4. Materials Data and Design Science for Materiel on Demand and by Design

Authors: William Benard, Ray Wildman, and James Snyder

4.1 Introduction

The ASPSM held 11–12 December 2018 entitled “Materials Data and Design Science” brought together research leaders in both materials design and design science to determine a strategy for integrating and operationalizing research in materials and design science toward on-demand and by-design high-performance materiel for the warfighter. The meeting drew broad representation from academia, the DoD, and industry, included large defense contractors, successful Silicon Valley startups, and the Defense Advanced Research Projects Agency (DARPA). A key takeaway was that the materials design and component design communities are not currently closely integrated due to the shear complexity of the two domains.

In order for the domestic material and component design communities to produce the most advanced materiel possible for the future warfighter, the consensus was that the research community needs to

- develop shared design software language and tools to efficiently describe constraining requirements and optimize performance, which can be easily integrated into complex workflows and advanced design architectures;
- advance understanding of multi-parametric feedback across time and length scales to drive efficiency of characterization and optimization;
- develop accurate and scalable models of complex multifunctional material physics and interfaces to enable effective design of multimaterial components;
- develop a modularity strategy to partition complexity using domain-specific statistical depth, ultimately enabling robust design of critical elements; and
- cultivate workforce software and big data skills and materials and design expertise to advance design science.

The DoD should lead by establishing a tri-service design automation framework to provide the critical foundation to seed the development of compatible software language and tools across the domestic research community. This design automation framework has the potential to serve as an integrative knowledge construct to enable us to rapidly field the most advanced materiel, adapt and adjust to emerging threats and conditions, and efficiently assimilate new technologies.

Opportunities were identified for accelerating the transition of new technologies through disruption of the current engineering design process. Additionally, the need to effectively share materials data was reaffirmed to help address the high-dimensional sparseness of materials data. The Army must continue to leverage and support materials data archiving efforts like the Materials Genome Initiative (MGI) and build design tools thereupon.

4.1.1 Background

The significant investments in materials and manufacturing research over recent decades have trended to increasing emphasis on modeling to drive understanding and improve experimentation efficiency. This approach has taken advantage of the reduced cost of computation (via Moore's law) and helped balance the rise in cost and complexity of experimentation. Despite advances in computational capabilities, we are still far from capturing relevant chemistry and physics where there is significant complexity. With the advent of Big Data, MGI has endeavored to make all federally funded materials research data accessible to all in support of data mining. The emergence of these rich data sets combined with new data science tools provides additional pathways to understanding complex interrelationships, reducing complexity, and augmenting known chemistry/physics to enable new abilities for rapid advancement of materials and manufacturing technologies.

In tandem with these developments, additive manufacturing is vectoring to a point-wise capability for mixing materials and modulating material properties almost arbitrarily within a monolithic component. This significant reduction in design constraints is extremely powerful in terms of producing components with extraordinary performance, but optimal solutions (especially for multiphysics applications) may be highly nonintuitive and complex to identify or define.

To accelerate the pace of technology development and deliver new capabilities to the warfighter, the Army must accept and address the key bottleneck limiting the adoption of advanced technologies: complexity of design.

4.1.2 Army Need

The Army acquisition enterprise is structured to deliver the most robust and resilient solutions possible. The goal is admirable: to minimize the variability and risk where we can for Soldiers who face significant uncertainty and risk in the execution of their duties.

The tyranny of excessive testing has been exacerbated by advances in understanding of failure modes. As we understand more about failure modes, we test more. As equipment becomes more sophisticated, we test more. The corollary

is that for constant development effort, the burden of testing increases. This constrains the rate of technological advance.

The consequences are twofold:

- 1) The cost of new materiel is disproportionately high in both time and dollars.
- 2) We fail to take advantage of new technological advances in a timely manner.

Our adversaries are not as conservative. They learn from our mistakes and are willing to take risk in materiel development. That risk is translating into adversarial overmatch.

We have not been remiss in our development of new materials and technologies. Nor have we failed to share these advances with the materiel development community. The inability to operationalize these advances is often the result of insufficient knowledge for design and the absence of capable design tools.

We need to advance how we design materiel. We need to develop tools to manage complexity at the system and subsystem level. This will enable digital testing so as to provide some relief from physical testing. Furthermore, system understanding developed from models can then be used to design efficient physical test vectors.

Component design is the process in which materials and mechanics research is operationalized. Component and ultimately platform designs should be embodied in highly automated design workflows such that the design can easily be recomputed to take advantage of new advances in materials, mechanisms and processing; rapidly adjust to emerging threats; or address new failure modes. Critically, the modules we assemble into workflows are persistent operationalized embodiments of the knowledge developed by the materials S&T enterprise, which endure long beyond the tenure of the creators.

For example, in the high-end microprocessor world, a human has not had a direct hand in laying out circuits in decades. Humans code in high-level requirements and architectures use sophisticated abstractions, which are compiled to produce multilayer device computer-aided design using a myriad of tools and models. The result is extremely complex and high-performance devices that would take decades to produce without design automation. This is possible due to extraordinary characterization of materials and process, and a refined ontology.

4.1.3 ASPSM Overview

This ASPSM sought to explore the challenges and opportunities of constructing integrative software architectures that build on advancing materials, process, and physics models to automate design of high-performance multiphysics components and access the expanded design space offered by flexible manufacturing. The questions used to seed the discussion were as follows:

- Can we adequately automate material and process model development from large data sets for design application?
- How do we build integrative architectures to leverage materials, process, and physics models and understanding to compile optimal multifunctional designs?
- How do we intelligently manage the inherent sparsity of high-dimensional data sets and the complexity of multiscale modelling?

The key themes and goals pursued were to 1) identify research questions and methodologies for capturing materials research knowledge (not just data) in an actionable/automatable persistent, pervasive form; 2) identify research questions and frameworks to enable high-performance lean design-on-demand for agile manufacturing; and 3) minimize the verification and validation burden for new components through high confidence in design as well as process modelling and analysis.

4.2 Vision and Obstacles

The first session of the meeting focused on the vision for the ASPSM premise. The participants were asked to consider the value proposition of integrated materials, process, and physics models to enable high-performance lean design-on-demand. In addition, many obstacles were identified and discussed.

The discussion focused on the following general themes:

- How would we design differently given improved tools?
- How would we manufacture differently?
- What foundational scientific advances would we need?

4.2.1 How Would We Design Differently Given Improved Tools?

In the near term, improved tools will certainly lead to incremental advances in our ability to design components and materials; however, the challenge of the ASPSM was to identify longer-term concepts and benefits of highly efficient and complex

design tools. What follows represents concepts that may not be attainable in the near future, but only with significant investment of resources.

4.2.1.1 Point-Wise Material Property Design Freedom

The farthest-term, most powerful design space was understood to be the point-wise definition of a component composition and microstructure in near real time. Integrated multifunctionality was considered to be valuable. This led to the proposition of an interesting conceptual design challenge to frame thinking: How would one approach the design of a highly integrated single multimaterial component system that is comparable in complexity to a living organism?

Relatedly, it was noted that the design optimization community should begin to move away from bulk homogenous property design in isolation. Materials design tools need to develop materials for design and application—not just myopic key properties, but all properties that will impact ultimate component performance. One popular approach (mostly to ease computational burden) is to design bulk material properties using optimization methods (e.g., design a composite material with negative Poisson's ratio, maximal stiffness, maximum conductivity, and so on). However, this approach may ignore the overall design objective of a larger-scale component. Further, integration of these optimized composite materials into a full-scale component may be difficult and may ultimately lead to degradation of the optimized properties. The goal should then be to optimize at this smaller material scale, but only with respect to objectives defined on the macroscale. For example, it is more important for bone scaffold to encourage bone growth rather than to provide simple mechanical stiffness. And as another example, the materials that make up the helmet of a helicopter pilot must be hard and heavy enough to protect the head from blunt trauma, damp ambient sounds, and vibrations, yet light enough to carry electronic components, and remain compact enough to enable pilot mobility. This coupling will of course increase the computational burden during design but hopefully add the benefit of increased overall system performance.

In order to develop more advanced design tools, it was widely agreed that a new language is necessary to efficiently describe the problem set and potential solution space. Language-based approaches in multiphysics simulation have proven very flexible and yielded interesting results. For example, the data storage requirements alone of a multiscale component definition could be prohibitive. A topology optimization problem can easily eclipse millions of unknowns at the macroscale, thus introducing subscale material descriptions at each unknown, quickly compounding the problem size. A more compact design language will reduce this burden not only for data storage, but for optimization as well.

4.2.1.2 Novel Objective Functions

As manufacturing freedom increases and optimization methods become more sophisticated, there is not only an opportunity, but also a need to incorporate objectives exploring the trade-offs between cost and manufacture time of components. The most obvious and straightforward cost model is simply to use the cost of materials, though there may be opportunity to implement sophisticated cost models that account for economies of scale, life cycle, and logistics costs. Another example is postprocessing requirements. Different manufacturing techniques and material combinations may have different postprocessing requirements (such as heat treatment), and postprocessing represents another cost/performance objective.

In addition, there was discussion of how to incorporate “soft” objective functions, or objective functions without clear mathematical definitions such as tactile feel and intuitiveness of use. Often, adoption of a component may be driven by how it feels and how easy it is to use. For example, any system in which a human is responsible for control, such as a vehicle, requires some type of control interface, such as a steering wheel and pedals. Modern cars use power steering to ease control and improve usability of a steering wheel, while in an abstract optimization setting, direct mechanical linkage of the steering wheel to the wheels may be optimal. Indeed, power steering is suboptimal from a system-level energy usage perspective, since additional power is required to operate the power steering pump. It is thus important for any design algorithms that are attempting to design systems with human operators to consider usability.

A separate but related issue is that of design complexity: Is it desirable to ultimately generate designs that are fully understandable to humans? This may aid in the acceptance and testing of computer-generated designs, though it may be difficult to incorporate this concept into a design language/optimization algorithm. As problem complexity scales, the ability of human intuition to meaningfully inform the internal workings of the design the process will wane. However, the design process still needs to be intuitive to make sure we accurately translate need into component.

Another interesting concept was that of designs that fail gracefully. While, ideally, components and devices should never fail, this is an inevitable outcome given enough time in service. With advanced models of failure, we could then begin to design devices that have a failure mode that is not catastrophic. For example, composite materials may fail catastrophically under certain loads, while steel exhibits ductile behavior before its ultimate failure. A useful design objective may be then to design components using composite materials, but fail in a way similar to steel. More generally, the concept of addressing rare but catastrophic events was

discussed. This may require a design algorithm to automatically identify overly sensitive loading conditions during the optimization process and eliminate them.

Finally, an interesting concept is that of a real-time objective function or dynamic design—for example, a responsive physical phenomenon like muscles growing. At a minimum there is interest in taking advantage of transients of manufacturing into design properties.

4.2.1.3 Multiple Objectives

Practical design problems will frequently involve trade-offs between multiple objectives. A simple example is the trade-off between mass and stiffness of a load-bearing component. Unconstrained, the optimal solution for a load-bearing component is to simply add more mass, and the design problem only becomes interesting when the available mass is limited.

As additional objectives are identified as being important, the need for multi-objective optimization techniques will increase. Solutions of multi-objective optimization problems are not a single design, but a suite of designs representing the various trade-offs between two or more conflicting objectives. For example, for a problem with two objectives, designs can be identified as a point in a 2-D objective space, with each objective represented by one axis. The result of the optimization would be a set of designs along a 1-D curve, hopefully separating inferior designs from infeasible designs. Increasing the number of objectives increases the dimension of the objective space and leads to difficulties in ultimately visualizing and choosing the desired designs for manufacture. Thus, it was envisioned that this process could be guided by an AI that helps pare down the number of optimal designs.

4.2.2 How Would We Manufacture Differently?

As additive manufacturing advances and gives unprecedented control over material properties at small scales, it will become even more important to pair advanced design techniques with advanced manufacturing techniques. Otherwise, significant performance benefits may be lost by simply using traditional design. Further, advances in sensor feedback will be extremely useful for informing models used in optimization.

Ultimately, design and manufacture must be tightly integrated to improve qualification and reduce failures during manufacture. An important concept will then be virtual testing built into the design process; however, there are significant challenges in translating between physical and virtual experiments. Representation is difficult—existing tools are very limited, so we need to develop surrogate models

that accurately interpolate across multifunctional and multifidelity domains, as well as bridge between physical and virtual experimental results. These models need to have uncertainty quantification (UQ) built in.

4.2.2.1 Agile, Threat-Responsive Manufacturing

Advances in additive manufacturing may also improve turnaround time for manufactured components. This will allow us to quickly design and redesign on the fly to adapt to changing threats. Agile manufacturing provides an incentive to incorporating manufacture time as an objective in our design optimization methods. There may be times in which the time to manufacture is more important than cost or other factors.

There are some inherent risks to fast design and manufacture, including the risk of using unqualified parts. These risks must be mitigated using advanced qualification techniques discussed herein. For example, new designs may be confined to more simple parameterizations of existing designs, and design algorithms will be aware of the tolerances necessary to maintain a qualified part.

4.2.2.2 Sensor Feedback

Sensor feedback must be factored in as early as possible to drive efficiency and reduce complexity. Sensing embedded across time scales should provide as timely feedback as possible to filter the solution space or provide corrective input:

- Feedback in manufacturing to inform processing
- Post-manufacturing verification and validation (including test development, design of surrogate test articles, and nondestructive evaluation)
- Embedded sensing and lifetime monitoring

Further, data from sensors could be used to generate models used in the optimization process.

4.2.2.3 Multimaterial Printing and Interfaces

Most current additive manufacturing technologies are restricted to one material per component, though that may change in the near future.

Interfaces between materials represent challenges and opportunities. There are significant challenges in accurately modeling interfaces in an efficient manner; however, it is undoubtedly possible to exploit material behavior at interfaces to generate better-performing designs.

4.2.3 What Foundational Scientific Advances Would We Need?

The scale of the potential design space was the primary technical challenge the group sought to engage since naïve incorporation of multiple materials, manufacturing methods, and objectives leads to a combinatorial explosion of the search space, resulting in high-dimensional, highly nonlinear optimization problems. The key concepts proposed to address this were multifidelity modeling approaches that vary resolution for expedient refinement of the problem space; intelligent partitioning of the problem into easily tractable components; and embedding feedback cycles at all levels for rapid candidate filtering and/or adjustment. Another foundational concept was the need to archive and share data and results to continuously increase the resolution.

To address the extraordinary scale of the full design space, we need to develop a quantitative understanding of scale and resolution—that is, when do we need to resolve properties as a function of microstructure as opposed to safely using lower-fidelity models? For example, while objective functions are mainly defined in terms of computational physics models (typically finite elements), data-driven models derived from experiments may be more efficient and possibly necessary as new materials and manufacturing techniques are invented. In support thereof, we also need to understand what is efficient—which tasks should be precomputed versus computed on demand.

Cost is fundamental—monetary, computational, and logistic. As such, we must advance frameworks for resource sensitive computing, problem scaling, and partitioning to use available computing resources most efficiently. Ideally, the overall problem decomposition and prioritization would be informed by a computation, confidence, and logistic budget.

Robust solutions will be important to aid the qualification process. Indeed, by design, optimization will generate components tuned to a specific objective, possibly at the detriment of other unstated but necessary qualities. Stable manufacturing paradigms should be adopted to enable us to prioritize robust solutions. Additionally, this understanding must be extended to enable high confidence development of parametric design.

As mentioned previously, efficient search space exploration is key to design science. It is important to develop software agents to ensure efficient knowledge capture, cataloging, and recall so it is not lost and is available for appropriate reuse. This is no trivial task, as ideally, no simulation would need to be repeated if, for example, a search algorithm generates a duplicate design at different points in the optimization process. Cataloging simulation results may require large amounts of data storage and further, it is not immediately clear how to efficiently map designs

to simulation results as designs are typically composed of millions or billions of design parameters.

Additional considerations, including data space, are highly dimensional and conversely sparsely populated, and similarly, the understanding of opportunity space is sparse. Architectures are needed to translate the requirement into specifics for a component while factoring in design for manufacturing and address the considerations that materiel lives forever and materials live forever (recyclability). Tools are required to identify the materials that fulfill the design need, determine the resolution of physics modelling, and consider whether materials and processing are compatible. Ideally, designs should move beyond uniform microstructure to gradients, interfaces, and mesostructure.

4.3 Pathways and Opportunities

The second and third sessions of the meeting focused on how to achieve the vision through near- and long-term breakthroughs, followed by the identification of gaps and opportunities to address Army challenges. The three focal areas for discussion were identified as Tools and Design Language; Modularity Strategy; and Feedback and Intelligent Autonomy.

4.3.1 Tools and Design Language

4.3.1.1 Design Language

The concept of a shared design language resonated strongly with the participants, primarily as a way to ensure consistent human understanding, but also extending into a design software language to enable high-level problem definition. As is evidenced throughout this report, the need for precise problem definition in a highly dimensional problem space necessitates tools that offer accurate high-level abstraction for system-wide perspective without a loss of resolution in execution.

The creation of a design software language assists in establishing modularity such that continuous parallel development of key functions (e.g., optimization functions) is possible. Additionally, it opens the door to efficiencies of code reuse for commonly used design constraints—for example, a module may describe the environmental operational constraints for an Army ground vehicle to include environmental temperature range, vibration, abrasion, and so on, while another describes the properties of the available design materials. These could then be reused for the design of all subsequent ground vehicle components and platforms. Creation of a design grammar will rapidly accelerate the development and refresh rate of design workflows.

This approach also lends itself to the incorporation of advanced visualization tools necessary to develop intuition and assist in driving a robust design process. Additionally, modules can be developed to guide manufacturing with concepts of how the component came to be, how performance is achieved, and what sensitivities might exist in manufacturing. Furthermore, visualization and other methods of interfacing with data are anticipated to be critical to enabling rapid human-in-the-loop decision making as both design complexity and design space increase.

There is significant opportunity to embed AI in design software modules for multiphysics and multiscale modelling. It was thought that the complexity of the design process may be overwhelming for many users, and thus an AI aide would be most useful to guide the designer through a series of questions about their design goals. Another opportunity may lie in communicating with a human to understand and respond to design preference and add constraints and optimization priorities during nonintuitive design review, rather than using a strictly imperative or declarative design language.

4.3.1.2 Solution Space Complexity Management

As mentioned, the incorporation of variable materials and their microstructure, manufacturing methods, and parameters, along with macroscale design into an optimization framework, greatly expands the dimensions of the search space. The development of tools that can efficiently pare and search these spaces will be of paramount importance.

One approach will be variable fidelity models that trade accuracy for efficiency when needed. While variable fidelity models work for systems that scale in a straightforward manner, they do not appear to work as well for stochastic, combinatorial, or discontinuous design spaces. There is then a need to develop tools to detect, classify, and accommodate these situations.

Partitioning of the problem isolates elements into smaller more tractable domains. Additionally, the solution space can more easily be screened to remove unsuitable candidates. Consequently, significant effort has to be assigned to problem definition to ensure that the solution space pursued serves accurately the need and intent. For example, we need to understand the risk tolerance of application and trade explicitly with opportunity cost in situations when

- moderate risk is not worth assuming if it does not translate to savings; or
- significant risk may be worth pursuing if the cost of having nothing is extraordinary.

Similarly, the design process should consider the full design space, which needs to be adequately described, and should be devoid of the inherent assumptions that occur in traditional design such as properties inferred but not stated in materials selection. For example, general classes of performance requirements should be established for materiel, including temperatures that Army vehicles need to survive (storage and operation). These classes of requirements must be codified to guide material selection, rather than limiting artificially the selection of materials to those that are known to work for a wide range of unstated performance requirements. Explicit capture would help identify failures based on bad or missed assumptions. Additionally, placing the full set of bounds on what the solution could be for a given opportunity (materials and machines available, performance envelope, etc.) pares down the potential solution space.

4.3.2 Modularity Strategy

The development of guiding principles for problem decomposition was considered a foundational need by the meeting participants due to the high dimensionality of design spaces accessible by manufacturing. Fundamental to implementing modularity is the need to understand the benefits and caveats of various trade-offs; for example, consider the cost/benefit of full material and geometry co-design versus independent but coupled optimization processes. Modular development offers the promise of piecewise advances, allowing for rapid and continuous accommodation of changes, such as to take advantage of superior new materials or optimization methods. Modularity in system design further mitigates the impact of failure in increasingly complex and multifunctional component designs by enabling rapid and targeted replacement of the affected component without compromising the rest of the system. The need to partition complexity into tractable problems, however, will result in some complexity driven to interfaces between design modules.

Initially, the extreme programming approach may provide a viable route to modularity—that is, only solve what we need to solve, keep the modules simple where possible, and understand that modulation and deviation from what is standard comes with increased verification and validation burden. There is a fundamental tension, for example, between robust data sets and materials design/customization. Custom materials design has the potential for higher performance, but this is tempered by the high additional characterization burden. Ideally, a modular approach will enable some efficiency gains through potential for precompilation and computation reuse. New Ashby domains should be sought. Additionally, new materials and process compatibility databases need to be established and maintained.

The workflows developed should be materials agnostic, so that advances in materials design can be easily refactored. Similarly, architecture should be abstracted to seamlessly take advantage of improvements in computational capabilities. Much of the necessary efficiency work will be contingent on the computational resources we can expect in the future: Quasi-Moore's law improvements? Massively parallel quantum computing? Stagnation? Ultimately, a modular approach is more naturally adaptable to each situation.

4.3.3 Feedback and Intelligent Autonomy to Drive Scaling

Another key approach to aid in the efficiency of solving these complex high-dimensional optimizations is to apply learning immediately—that is, rapidly pare down the massive design space by removing invalid and poorly performing candidate spaces as soon as they are identified and retaining as much information as possible to avoid costly forward solutions. Additionally, as new information becomes available, it should be considered to full effect. Immediate feedback from failures adds intelligence to the system and advances design. Multiscale feedback from production, testing, and operation, as well as by engaging multiresolution model architectures, should be used to rapidly refine and verify designs. Reduced order models help accelerate solutions by expeditiously uncovering promising directions for computation resource allocation. This is a potential application for Artificial Intelligence/Machine Learning (AI/ML)—to produce efficient models that serve to interpolate across models.

In support of automating design workflows that leverage big data, additional tools need to be developed beyond simulation, modeling, and optimization. Tools are needed to manage the complexity of defining point-wise materials properties (voxelization) and determine what the relevant properties (e.g., impedance, transparency, strength, and so on) necessary are for both fabrication and operation. Furthermore, they need to consider the impact on the voxel of both fabrication and operation. Tools are also required to marshal large data sets in order to minimize the human effort of data acquisition, as well as to ensure the integrity and completeness of the data. Data mining and communication tools are necessary for locating and identifying archived data, results, and models; and market places are necessary to ensure they are used to full effect.

In order to keep design problems tractable, it is expected that significant in situ testing will be deployed to verify approaches and reduce uncertainty. Again, efficiency is key. For that reason, workflows should deploy low-cost, high-throughput testing, nondestructive and virtual testing, and progressive testing (frequent screening throughout the design process, both physical and in silico, and abandoning nonproductive alternatives as soon as they fail a test). Furthermore,

approaches should be developed that adaptively modify the design-of-experiments to understand failure of a test. UQ is essential to automating design workflows. UQ has a relatively high cost and so should be incurred only when necessary or efficient. It does, however, serve as a critical indicator of how best to distribute computational effort. Additionally, tasks that advance understanding and/or knowledge development should have elevated priority in the assignment of computational effort.

Additional considerations in workflow construction are robustness (insensitivity of process to variability to achieve repeatability); logistics (reduce diversity of feedstock choice due to logistic effort); and factors associated with the entire lifecycle of the part such as recyclability. Automated design workflows should consider the complete design problem, so that the final product embodies the full benefits of optimization rather than requiring significant postprocessing to address additional constraints. Postprocessing often reduces, if not outright defeats, the improvements afforded by optimization.

4.4 Conclusion and Recommendations

4.4.1 Summary

Throughout the meeting, it was clear that there has been much investment of time and resources into the disparate areas of materials data and design science. There has not been enough cross talk, however, to solve larger-scale, realistic design problems. Further investment in and development of advanced manufacturing methods that increase freedom and flexibility in production will necessitate design methods that can take full advantage of the increased freedom and flexibility in production.

The benefits of fully coupled and comprehensive data and design science are numerous, including (but not limited to) improved performance of components; agile/threat-responsive design; improved cost and manufacture time efficiency; design trade-off exploration; and complex function consolidated multimaterial components.

Several paths forward were identified. These are broadly grouped into tools and design language; modularity philosophy; and feedback and intelligent autonomy to drive scaling. The development of tools and a design language will be necessary for reducing complexity for the designer and allowing the designer to communicate intent in a straightforward manner. A modularity philosophy will be necessary to reduce complexity for the developers of the design and data methods. Finally, feedback and intelligent autonomy will be important for reducing the complexity

of the search space, allowing the design algorithms to generate meaningful solutions in a short period of time.

4.4.2 Recommendations

A significant investment in design science is required to leverage the full benefits of materials and manufacturing research. Investment has the potential to yield significant rewards in both the defense and commercial sectors but is unlikely to be realized without a critical seed community working with a common framework.

- Investment in design science should be driven by the understanding that the modules developed to populate design workflows are fundamental knowledge products. These knowledge products have the exceptional potential to be persistent, integrative, and immediately actionable. The successful development of knowledge architectures for integrative intelligence is fundamental to achieving enduring technical domination both on the battlefield and economically.
- Tri-service and cross-governmental coordination is essential to form an open framework with adequate scale to attract academic and industrial participation and investment. An open framework will allow domain-specific modules to be developed; integrated into design workflows; and reused in new design workflows. The existence of a common framework can serve as the foundation for module marketplaces to enable government, industry, and academia to request and supply specialized modules necessary for a design application. Proprietary efforts will not provide the requisite flexibility, nor support the unique design considerations for DoD applications, and are unlikely to scale to realize full potential. Ideally, an Office of Science and Technology Policy-lead national research initiative would be established for design—for example, a National Manufacturing Model, Data and Design Initiative.
- Treasure data today. The MGI is extremely valuable in establishing a data foundation for materials design. International materials data sources should also be indexed in support. A marketplace must be developed to prioritize and incentivize data capture, storage, and sharing. An explicit business model must be defined to ensure data can be acquired on demand and have the appropriate persistence based on value.
- Invest in materials and process module development to address the challenges of multimaterial synthesis and processing. Additionally, advance in-situ characterization tools and technologies for high-throughput screening of materials.

- Further investment is needed in computational tools to intelligently manage large optimization problems. Ideally, these tools will be capable of recognizing the available computational resources and scaling resolution to balance accuracy and computation time. The tools should further be capable of fully accounting for the available manufacturing methods and materials available and any cost or manufacture time constraints to ultimately generate designs representing optimal trade-offs of the design goals. Ultimately these tools will assist optimization efficiency by promoting workflows that incorporate simulated and physical test vectors to economically reduce uncertainty.
- Workforce development is a fundamental challenge in design science. It was observed in the meeting that the two vibrant research communities of component design and material design are largely isolated despite the downstream research impact being tightly intertwined. Both the defense and economic impacts will be significantly enhanced by developing a workforce able to work the seam and bridge the two fields.
- The proposed framework has significant potential for a holistic design of high-performance materiel but also provides the key elements for a digital twin for sustainment engineering. Similarly, the framework provides the tools to probe the impact to system performance of proposed or expected scientific advances. Use cases should be developed to understand the needs of these domains.

4.5 Acknowledgments

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4.6 Definitions

| | |
|--------------------|--|
| Component | Element of a system, typically produced monolithically. Alternatively called a “part”. In this treatment, no specific technical field or application is assumed (mechanical, electrical, etc.). |
| Voxelization | Defining the point-wise properties of a component. Traditionally, the variation in properties is a consequence of the manufacturing process; going forward, there is the opportunity to modulate the process to adjust the materials properties within a structure as a function of location within the component. |
| Objective function | A mathematical or computational representation of a design problem. The objective function is what an optimization method seeks to maximize or minimize (typically subject to one or more constraints) to give an optimal design. This is typically a computational implementation of the relevant physics, such as finite element analysis of continuum mechanics for maximal stiffness problems. |

5. Real-Time Learning, Knowledge Bases, and Information Retrieval

Authors: Brian M Sadler and Douglas Summers-Stay

5.1 Background

Future Army intelligent systems are expected to learn from a variety of experiences; interact with autonomous agents, Soldiers, and experts; and utilize and update stored shared information. Army autonomous intelligent systems are now progressing beyond simple levels of control and incorporating perception and higher levels of cognition. These systems require long-term memory that can be updated in real time, queried for inference and reasoning, and support Soldier–system interaction and semantic dialog.

Artificial Intelligence (AI) and Machine Learning (ML) now provide a toolbox of methods and algorithms that are being applied across a variety of Army applications—in particular, deep learning (DL) has provided significant advances in processing natural signals (vision, language). Data-driven DL requires a large to massive number of labeled examples for training, which is achieved in batch (offline) processing that is computationally complex. Meta-learning (learning to learn), or other approaches, seek to adapt DL and make it more general and flexible, but tend to continue to have heavy data requirements subject to the availability of prior models or specific and controlled application domains.

In addition to the developments in DL, recent progress in knowledge bases (KBs) and semantic-driven processing has also been significant. Graph-based KBs can be constructed from a large corpus, such as mixed-media, written text, and speech. These KBs can be queried in machine–machine and human–machine contexts and support intelligent dialog, such as Soldier–robot task collaboration. They can also be updated in real time and specialized for a variety of uses.

5.2 Objective

The focus of this meeting was to explore the underpinning science needed for future Army intelligent systems that combine autonomous control, real-time learning, and memory in the form of knowledge bases. This brought together experts in robotics and autonomy, DL for perception, semantic reasoning, and KB construction and querying. The autonomy and semantic KB research communities are largely separate, and a key goal of this meeting was to draw from both areas to consider

the cross-disciplinary intelligent systems issues and identify key research questions and collaborative multidisciplinary research areas.

5.3 Intelligent Systems

Figure 1 depicts the components of a potential future warfighter scenario that incorporates autonomy and knowledge bases into a communications network. On the “control” side are autonomous agents, robotics, and sensors, while on the “semantics” side are KBs, higher-performance computing assets, and human experts. It is a long-term goal to unify these components into intelligent systems that support and team with the warfighter. The workshop specifically focused on the autonomy and KB components, considering how these separate technologies and be unified.

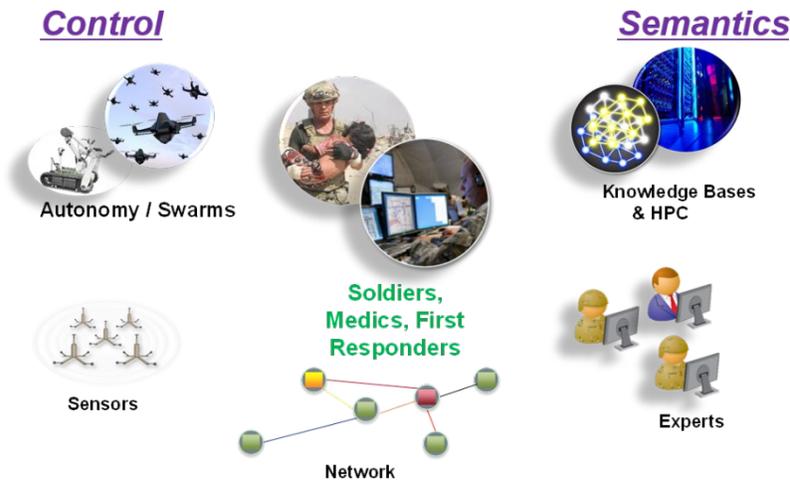


Fig.1 The components of a distributed intelligent warfighter system, combining autonomous agents with semantic KBs

5.4 Key Research Challenges

The workshop identified the following key research questions and challenges:

- KBs and autonomy
 - How can KBs provide long-term memory? What are unifying representations?
 - How to combine DL and KBs for intelligent systems?
 - What kind of KBs are needed for Army autonomous operations?
 - How can multiple agents learn and share KBs?

- What representations support efficient machine–human–KB interaction?
- How can iterative online learning and KBs be combined?
- Semantic reasoning and control
 - How can they be combined in an analytical framework?
 - Can the combination overcome the adversarial AI problem?
- Computation
 - What is the right mix of cloud, distributed, edge computing, and storage that supports Army tactical operations?

5.5 Semantic SLAM

Current work on semantic simultaneous localization and tracking (semantic SLAM) is an early step in this direction, combining traditional robotic-sensor-based SLAM with semantic information about the scene, such as object labels. An autonomous agent can reason about the scene as it explores and maps, bringing significant advances in the ability to create much more than a geometric picture. Envisioned more broadly, the ability to link and apply reasoning among geometry, mapping, and objects in the scene will lead to leap-ahead cognitive capability. This can be applied for threat detection, scene context, human–machine interaction, and a host of warfighter scenarios.

5.6 Conclusions and Recommendations

There was broad consensus that the potential unification of autonomy and KBs could have a significant long-term impact on future Army intelligent systems in a variety of settings. Dramatic but separate progress over the past decade has occurred in AI for autonomous control and robotics, as well as semantic processing and KBs. While these two research communities are largely distinct, there is a significant opportunity to create a new multidisciplinary approach to Army intelligent systems that has high payoff.

5.7 Recommendations

- Accelerate cross-disciplinary research spanning autonomy (especially but not limited to) robotics, and KBs.

- Further develop human–KB querying methods and link these with human–autonomy (human–agent teaming) research that includes machine–KB interaction.
- Accelerate graph-based and other formalisms to provide unifying analytical frameworks that lead to mathematical bridges between autonomy and KBs.
- Develop processing architectures for intelligent systems that combine autonomy and KBs, leading to experimentation and fundamental understanding of architecture tradeoffs.
- Further incorporate learning (AI and ML) methods into building KBs and facilitating their application in intelligent systems.
- Consider the adversary problem, such as counter-autonomy, and how links with KBs can lead to more robust and resilient autonomy.
- Consider a broad array of KBs for different applications and develop methods for cross-KB querying and collaboration in the larger context of autonomous systems.
- Consider how to update KBs for continuous learning.

5.8 Workshop Presentations

Overview

Dr Brian Sadler, ARL

Area 1: Knowledge Bases

Prof Xifeng Yan, University of California, Santa Barbara

Prof Huan Sun, Ohio State University

Prof Yu Su, Ohio State University

Area 2: Representations

Dr Douglas Summers-Stay, ARL

Dr Graham Bent, IBM

Dr Rod Rinkus, Neurithmic Systems

Dr Volkan Ustun, USC Institute for Creative Technologies

Area 3: Autonomy

Prof Yezhou Yang, Arizona State University

Prof Nikolay Atanasov, University of California, San Diego

Prof Harish Ravichandar, Georgia Institute of Technology

Prof Peter Stone, University of Texas, Austin

List of Symbols, Abbreviations, and Acronyms

| | |
|----------|--|
| 1-D | one-dimensional |
| 2-D | two-dimensional |
| 3-D | three-dimensional |
| AI | Artificial Intelligence |
| ASPSM | Army Science Planning and Strategy Meeting |
| BZ | Belousov–Zhabotinsky |
| CCDC ARL | US Army Combat Capabilities Development Command Army Research Laboratory |
| CONOPs | concept of operations |
| DARPA | Defense Advanced Research Projects Agency |
| DL | deep learning |
| FY | fiscal year |
| KB | knowledge base |
| MGI | Materials Genome Initiative |
| ML | Machine Learning |
| MTBF | mean time between failure |
| NASA | National Aeronautics and Space Administration |
| NEEC | nuclear excitation by electron capture |
| R&D | Research and Development |
| RTG | radioisotope thermoelectric generator |
| S&T | Science and Technology |
| SLAM | simultaneous localization and tracking |
| SMET | Squad Mission Equipment Transport |
| TE | thermoelectric |
| TES | thermal energy storage |
| TPV | thermophotovoltaic |

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FCDD RLS
WILLIAM BENARD
FCDD RLS DE
J J CARROLL
C J CHIARA
FCDD RLR EN
S STANTON
FCDD RLR PC
D POREE
FCDD RLV
B GLAZ
B H PIEKARSKI
B M SADLER
FCDD RLV A
J L SHUMAKER
FCDD RLV V
F GARDEA
FCDD RLW MB
R WILDMAN
FCDD RLW MC
J SNYDER