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Report from Materials Discovery for Extreme Environments Workshop

by Scott Schoenfeld, Christopher Haines, Philip Goins, Debjoy Mallick, James Snyder, Joshua Orlicki, and Sikhanda Satapathy

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14. ABSTRACT

The US Army Combat Capabilities Development Command Army Research Laboratory hosted a virtual workshop 27–29 October 2020 to discuss new concepts for accelerating discovery of materials for extreme environments. This workshop brought together a diverse group of academics, researchers, and practitioners with expertise in theoretical, computational, experimental, synthesis, and processing aspects of materials science and engineering germane to ballistic sciences. Presentations and subsequent discussion focused on elucidating technical gaps, as well as proposed approaches to address these challenges. Recurring topical areas included high-throughput material science, the integration of artificial intelligence, to include the criticality of rule (physics)-based models, uncertainty qualification, and the challenge of applying these approaches to high-strain-rate and high heating-rate environments.

15. SUBJECT TERMS

high-throughput materials science, data-driven materials science, materials for hypersonic applications, materials for armor/antiarmor, machine learning (ML) optimization of materials

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Executive Summary

The 2018 *U.S. Army Modernization Strategy* (AMS) report to Congress[*] introduced the Army's materiel modernization priorities, while the 2019 AMS[†] expanded the Army's approach beyond those six priorities, outlining a more holistic approach to enduring objectives and introducing long-term research priorities across the science and technology enterprise. The focus of these objectives is to provide unity of intent across the enterprise as we recognize an era of increasing scope and accelerating pace of science and the requirement to incorporate these innovations more rapidly than our competitors.

Within the Army science and technology enterprise, the US Army Combat Capabilities Development Command Army Research Laboratory is chartered to conduct disruptive foundational research, engage as the Army's primary collaborative link to the scientific community, and interface to shape future fighting concepts. We crystalize these ideas and the impetus to perform these functions at the pace of innovation as a mandate to "Operationalize Science for Transformational Overmatch". More simply put, we seek to accelerate discovery and move discoveries to the Warfighter faster than anyone else.

We held the 2020 workshop on Materials Discovery for Extreme Environments to focus on the confluence of two outstanding research priority areas at the intersection of materials research and ballistic applications; namely, the need for next-generation materials for terminal ballistics (materials by design for protection overmatch[†]) and hypersonic flight[†] (materials to withstand high heat, ablation), and to explore ways to accelerate discovery of high-performance materials in these extreme environments. The workshop was structured to examine the current approach to materials by design; namely, the methodical evaluation of materials structure, architecture, and design for specialized extreme environments and evaluate emerging and promising data-driven approaches that could accelerate the pace of this design cycle.

Major Findings:

- The Edisonian approach (i.e., trial and error) to research has resulted in slow, incremental advancement in materials science. The advent of Integrated Computational Materials Engineering and Materials by Design

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[*] Report, submitted to the congressional defense committees, marked as FOUO. 2018 April 30.

[†] *U.S. Army 2019 modernization strategy: investing in the future*. https://www.army.mil/e2/downloads/rv7/2019_army_modernization_strategy_final.pdf

has significantly advanced the field. While not entirely deterministic, these methods remain strongly rooted in rule-based but science-driven numerical methods.

- Data-driven approaches to discovery of new patterns (machine learning [ML]) are promising but will require volumes of data unavailable through conventional ballistics or current materials science. The volumes of data required will drive entirely new high-throughput experimental approaches; uncertainty will permeate these approaches.
- ML will permeate an optimization workflow that integrates high-throughput synthesis, characterization, and processing of materials while relaxing the reliance on costly high-precision experiments and slow, computationally intense, physics-based numerical methods. However, we are still quite early in the development these tools and techniques.
- The data management (hardware, software, and network) required for ML-based optimization will be extensive. This should be a major consideration in designing the optimization framework and building collaborative processes that will result in discovery of new materials.

1. Introduction

The US Army Combat Capabilities Development Command Army Research Laboratory hosted a virtual workshop 27–29 October 2020 to discuss new concepts for accelerating discovery of materials for extreme environments. This workshop brought together a diverse group of academics, researchers, and practitioners with expertise in theoretical, computational, experimental, synthesis, and processing aspects of materials science and engineering germane to ballistic sciences. Presentations, and subsequent discussion during breakout sessions, focused on elucidating technical gaps as well as proposed approaches to address these challenges. Recurring topical areas included high-throughput (HT) material science, the integration of artificial intelligence (AI) to include the criticality of rule (physics)-based models, uncertainty qualification, and the challenge of applying these approaches to high-strain-rate mechanical property measurements.

Multiple National Academies studies[1–3] have shown that the Edisonian approach to R&D (i.e., trial and error) has resulted in slow, incremental advancement in materials science. The advent of Integrated Computational Materials Engineering (ICME) and Materials by Design has allowed the field to take a step in the right direction, but these rule-based methodologies only represent a portion of available AI techniques and really only address the material design phase of the process. What is needed to accelerate materials discovery (and subsequent integration) is a more comprehensive methodology that not only addresses material design, but also considers HT approaches throughout the development process (e.g., synthesis, process, and characterization).

AI (rule-based and ML, together) presents powerful new tools for exploring an information landscape in ballistic materials design and discovery. Such approaches present considerable opportunity in exploring new frontiers for materials used in ballistic applications, especially when coupled with new approaches that allow larger and richer data sets, computational tools, and data infrastructure for collaboration. Broadly, AI/ML can be used to augment individual steps in the synthesis–processing–characterization pipeline, be used to bridge behaviors in length-scales from prototype materials to applications of interest, and be used to guide a broader research loop.

Advances in synthesis, modeling, and characterization will greatly advance our ability to exploit monolithic materials in extreme environments. However, there is a need to contemplate how the capabilities of additive manufacturing and other processing techniques can be used to evaluate materials that exhibit spatial variations in composition and anisotropic characteristics and contain interfaces among multiple materials. The parameter space expands exponentially as these variables compound the system inputs, but truly advanced materials' performance will likely depend on an integrated systems-level approach to materials design.

Application of ML toolsets is viewed as necessary to achieve accelerated discovery of new materials for application in dynamic (impact, thermal, and ablative) environments. ML toolsets and software exist but may need to be adapted for the specific requirements of materials discovery and design. Full exploitation of the ML approach will certainly require extension and further development to focus on proof-of-concept for material classes of interest in ballistic application. This could be achieved within a generalized and scalable framework that supports rapid, robust, and trusted data exchange. New tools to consolidate data and improved HT workflow will require specialized approaches to transient phenomena (e.g., shocks, heating, localized deformation, and failure). ML models that incorporate these phenomena will critically rely on physics-based models that target key mechanisms. Critical (targeted by ML approaches) physics models may require further development; ML offers opportunity to consolidate much of these physics into fast-running analytic frameworks compatible with the HT approach and may be used to guide autonomous systems for HT characterization of transient phenomena.

Autonomous decision making is critical to successful implementation of closed-loop material discovery. The appropriate development and integration of machine-directed decision making depends on defining input and expectations of output for each stage of the enterprise. Stages may comprise material synthesis, processing, and/or characterization, as well as models to connect and inform these stages, but will necessarily require HT of information. ML may be considered as a central guiding system or locally guiding (within any one stage) system or for extracting information from individual stages to iteratively direct additional actions. How ML is employed can depend significantly on the nature of data output and maturity of tools, which can differ substantially across the enterprise and be challenged by low-volume or sparse data. Active learning schemes and the like are expected to be important to guide the iterative research loop.

A robust collaborative mechanism among government laboratories, academia, and industry is crucial to leverage investments made by the different organizations, accelerate the discovery of new materials, and transition them to the Soldier. To advance the design timeline, any collaborative research effort will involve many researchers who must efficiently communicate with each other across multiple disciplines and institutions. There are multiple approaches to vertical integration, and design of the collaboration must carefully consider the desired outcome.

In summary, the US Army's modernization priorities require materials that survive and perform in extreme environments: harsh military environments of high-acceleration launch and flight, high-temperature and rapid ablation, and impacts at very high velocity. The totality of these environments and accumulating requirements on future materials drives the imperative to consider an increasingly large number of constituent elements, structure, and properties. Discovery must now parse through billions of candidate materials to achieve highly specialized and transformational functions. This requires a data-driven approach, one that fuses HT materials synthesis and characterization with ML algorithms and closed-loop discovery automation. We consider three critical questions:

1) High-throughput synthesis, processing, and characterization for extreme environments: What scientific opportunities exist in the next 5 years, and what gaps must be addressed?
    a) What are the limitations to achieving HT synthesis and processing and rapid characterization of metallic alloys, ceramics, polymers, and composites for extreme dynamic environments?
    b) Where in the synthesis–processing–characterization cycle can the integration of AI best be exploited for leap-ahead advances?
    c) What challenges need to be overcome to introduce spatial variation in composition, anisotropy, and interfaces in material systems to go beyond monolithic materials?
2) Accelerated analysis, discovery, and design of novel materials for extreme environments: What scientific opportunities exist in the next 5 years, and what gaps must be addressed?
    a) What are the key challenges and barriers that must be overcome to apply ML toolsets for discovery of new materials for application in dynamic (impact, thermal, and ablative) environments?
    b) How will emerging ML capabilities be integrated with emerging multiscale models as well as HT synthesis and characterization to complete material discovery loops? What are key barriers that must be addressed in 2–3 years, 5 years, and more than 5 years?
3) What collaborative models will best increase the pace of innovation? How best to leverage resources and expertise across this enterprise? Consider opportunities for workflow to discover materials with leap-ahead performance in ballistic applications.

Workshop findings are as follows:

2. Question 1a: What Are the Limitations to Achieving HT Synthesis and Processing and Rapid Characterization of Metallic Alloys, Ceramics, Polymers, and Composites for Extreme Dynamic Environment?

Emerging methodologies such as ICME and Materials by Design have allowed scientists to rethink the early stages of a material's development life cycle by integrating computational models and simulation into the material design and selection phase. This allows researchers to very rapidly hone in on the most-promising composition space, but is just the beginning of the R&D cycle. To ensure HT materials' discovery, it is imperative that the accelerated pace continues through the synthesis, processing, and characterization phases. This poses significant challenges, as most existing R&D infrastructure is not designed for HT and/or automated processes. Arguably, the synthesis and processing of both metals and polymers is far more amenable to HT processes than ceramics and composites. However, the characterization of all materials classes suffers from being inherently slow. Select techniques (nano-indentation, scanning electron microscopy, etc.) have seen limited levels of automation, but the majority of high-fidelity characterization techniques will require adaptation to HT. In addition, note that conducting high-strain-rate mechanical property testing in a HT mode is going to be considerably more challenging than quasi-static testing.

2.1 Challenges/Gaps

- HT synthesis of thin films has been demonstrated; progress on HT synthesis of bulk materials is lagging; microstructure is likely to be highly dependent on particular processing method and variables.
- Successful examples of HT synthesis of metals (e.g., high-entropy alloys) and some polymers are far more common than ceramics or composites; methodologies are more mature in these classes of material.
- Most synthesis and processing techniques lack in situ diagnostics and/or characterization; additive manufacturing may lead here.
- Processing is the most challenging area of the three. In contrast to synthesis, processing maps are ill-explored and offer simple guidance, if any. There is no straightforward or unified way to represent/encode processing history. Processing techniques vary widely and are sometimes proprietary, based on industrial standards, especially in ceramics. Process models are often very basic (e.g., master sintering curves in ceramics). Processing approaches are

often in large serial machines (or specific industrial equipment) and require handoff from the synthesis platform.

- Consistency in processing methods and techniques is critical to ensuring microstructure evolution during bulk processing.
- Length-scale and correlation across scales in bulk materials will be highly challenging:
    - Small samples may not contain defects that dominate behavior of bulk material.
    - Mechanisms can change across scales (e.g., deformation modes and failure).
    - Sensitivity at-scale may depend on application (blast vs. hypervelocity, for example).
    - Optimization may require at-scale alignment between synthesis/processing and characterization/testing plan.
- HT materials characterization techniques that are clearly indicative of high-strain-rate mechanical behavior are lacking.
- There are clearly rate-limiting steps; accelerating one single step in the chain may not really speed research.
- HT leads to higher uncertainty. There are tradeoffs between speed and accuracy. We must account for human factor (operator biases). Sparse but information-rich experiments are common for lab-scale dynamic experiments.

2.2 Potential Approaches

- Size scale of the application will drive throughput of synthesis, processing, and characterization. These must be carefully considered so as to close gaps between scales.
    - Identify where thin film work is relevant.
    - Develop robust scaling laws. Need to relate small-scale (or even thin film) properties to ballistic response; should be robust across the synthesis, processing, and characterization efforts.
    - Develop bulk combinatorial techniques; state-of-the-art techniques include deposition, ball milling, and more.

  - Need to consider scale of synthesis as to be able to generate samples that meet requirements of the characterization suite (i.e., program cannot revolve around thin films when bulk samples are required).

- Need to mature predictive capabilities for properties to better guide synthesis.

- Identify surrogate measurements that correlate to high-rate events for the Army application. Current state of the art: nano-indentation, Raman, gas gun, cylinder expansion, laser shock, and micro-Kolsky. Also need to develop in situ methods to capture high-rate data.

- Clearly define a hierarchy of characterization/testing such that the high-strain-rate tests are only on a handful of elite candidate materials.

- Rate-limiting steps need to be identified and targeted during development of workflow.

- Leverage processing capabilities unique to Army in-house programs; these are specialized to Army requirements and ready to partner with industry.

- Remove the human bottleneck. Develop automated and/or autonomous characterization systems with controlled data quality and understandable pedigree. Areas ripe for development include the following: automated microscopy to assess morphology, Raman, Fourier-transform infrared, micro-ballistics, nano-indentation, and Kolsky bar.

- Must conduct uncertainty qualification across the entire process, as well as across scales.

3. Question 1b: Where in the Synthesis–Processing–Characterization Cycle Can the Integration of AI and ML Best Be Exploited for Leap-Ahead Advances?

AI and ML present powerful new tools for exploring an information landscape in ballistic materials design and discovery. Such approaches present considerable opportunity in exploring new frontiers for materials used in ballistic applications, especially when coupled with new approaches that allow larger and richer datasets, computational tools, and data infrastructure for collaboration. Broadly, AI/ML can be used to augment individual steps in the synthesis–processing–characterization pipeline, be used for scale-bridging to draw greater information from more-tractable experimental approaches, and be used to guide a broader research loop.

3.1 Augmenting Individual Steps in the Research Cycle

3.1.1 Challenges and Gaps

- Few ML tools are designed for materials applications; they are more often for very large data sets found in the technology sector.
- Data sets in materials science are comparatively smaller than most ML approaches.
- It is not yet known what scale of HT is necessary for AI/ML approaches.
- Data sets have unknown factors that introduce noise within and between experiments (operator error, as an example of the latter).
- Many individual experimental and computational steps are slow.

3.1.2 Potential Approaches

- Existing ML tools provide great capability. However, these are not yet adopted to materials discovery; there remains tremendous impact to the field with minimal retooling. Survey existing industrial processes and techniques for examples of process optimization.
- Develop physics-informed ML (by thermodynamics, kinetics, and practical limitations) unique for ballistic applications.
- Implement physics-informed ML and data-rich, non-HT experiments to offset smaller data sets and reduce throughput generation of data.
- Focus should be on high-throughput aspects leveraging machine intelligence to scan multi-dimensional space.
- Develop relationships between ballistic performance/high-strain-rate failure and properties more conducive to HT measurements (hardness, strength, etc.).
- ML can be used to improve data quality via noise removal, bias flattening, and more.
- Refining existing ML tools to match specific experiments in the synthesis–processing–characterization cycle may offer a low-risk solution for quality results.
- Automating steps using ML can help eliminate uncertainty introduced by human error or operator biases.

- ML can be used as a “lower-fidelity” stand-in while slow experiments or computational steps (such as density functional theory) are being completed simultaneously, improving research cycle efficiency.
- (Suggested) Develop limited-scale experiments examining traditional serial, HT-experimental, computationally expensive, and ML-streamlined predictions to correlate data quality and predictive quality of the various methods.

3.2 Connecting Approaches in the Research Cycle

3.2.1 Challenges and Gaps

- Application-scale HT synthesis, processing, and characterization are not yet feasible on the research program timeline.
- Relationships between experiments at different scales are not yet known within ballistics performance, and mechanisms are likely to change between micro-ballistics and application-level ballistics.
- Multi-scale models for applications of interest are not fully developed.

3.2.2 Potential Approaches

- ML approaches can be used to draw information from small-scale “lower-tier” experiments and connect to HT characterization experiments.
- ML can be taught to identify key relationships between easily measured “small-scale” properties and application-scale performance.
- Computational tools can be used to identify physical mechanisms that change across length scales.
- Inverting experiments with ML to expand from quasi-static to dynamic problems by connecting state variables with high-resolution experiments/computation.
- ML focus on transient phenomena (e.g., wave propagation).
- ML can serve as “connecting tissue” between multi-scale models or between experiments of one scale and models of another.

3.3 Research Cycle Guidance

3.3.1 Challenges/Gaps

- AI and ML are powerful tools but not expected to work perfectly.
- Data handling among experiments, researchers, and institutions is often disorganized and in disparate formats.
- There is significant overhead cost in moving samples, data, and the like between facilities, which introduces substantial delay in research progress.
- Direct information regarding performance requirements for ballistics materials is often highly constrained by the necessary security environment.

3.3.2 Potential Approaches

- AI tools that guide research loop can be used to identify critical regions to study based on uncertainty, validation, or expectation of high performance.
- Study high-dimensional property-performance space—an area in which humans are relatively limited.
- Active learning is a promising area that has already been demonstrated in a few limited “closed-loop” or nearly “closed-loop” research structures.
- Uncertainty quantification at every stage of synthesis, processing, and characterization can provide a big-picture look at materials coming through the design loop, preventing a buildup of uncertainty through the broader research pipeline.
- Developing common data formats will improve collaborations and allow more-cohesive collaborative research pipelines.
- Automation by a central AI for a research cycle enables automatic data transport and, in the case of one-roof research facilities with automation, may enable a seamless flow of autonomous experimental execution as well.
- Improve predictive models for identifying near-term and far-term candidate materials for ballistic application.
- Human–AI partnerships are found to outperform either human or AI acting alone in certain tasks, and may be true for materials discovery as well.
- Development of a persistent, cumulative database of materials knowledge permanently improves the odds of future leap-ahead discoveries as program matures.
- Using current body of data, the most-promising candidate areas can be identified.

- An AI framework can be developed that searches for materials with very detailed requirements for a specific application (in contrast to human researchers).

4. Question 1c: What Challenges Need to Be Overcome to Introduce Spatial Variation in Composition, Anisotropy, and Interfaces in Material Systems to Go Beyond Monolithic Materials?

The advances in synthesis, modeling, and characterization will greatly improve our ability to exploit monolithic materials in extreme environments. However, there is a need to contemplate how the capabilities of additive manufacturing and other processing techniques can be used to evaluate materials that exhibit spatial variations in composition and anisotropic characteristics and contain interfaces among multiple materials. The parameter space expands exponentially as these variables compound the system inputs, but truly advanced materials' performance will likely be dependent on an integrated systems-level approach to materials design.

4.1 Challenges/Gaps

- Nonuniformity of materials vastly increases parameter space.
- Design of spatial variability is complex, and a distinction between material development and macroscale design may not be possible. Spatial variation within a material may or may not be meaningful at the system scale. High-throughput synthesis and testing must be carefully crafted to the target application.
- Controlled processing of spatial variability remains challenging. Capability to synthesize/process anisotropic or graded materials at scales relevant to HT analysis may not exist, and may not be transferrable to scalable manufacturing approaches.
- Understanding of interfacial interactions and bonding is incomplete. Development of this understanding in the context of hypersonic and impact applications would be necessary to complement any data-driven design approach.
- Full-field imaging is emerging for high-rate events; however, resolution remains too low to capture relevant mechanisms in small samples.

4.2 Potential Approaches

- ML-driven models may help bridge between small-scales and bulk performance. Predictive models and physics-informed ML can be part of a strategy to understand the performance trades enabled by nonuniform composition as well as consideration of cost/benefit.
- Additive manufacturing is an opportunity to control spatial variability; techniques are promising and can deliver gradients in microstructure and composition. Suitability varies by material class, but there are certainly opportunities to explore metals and shape memory alloys.
- Thin films as small-scale surrogates for testing proof-of-concept for ballistic applications are possible. Techniques for evaluation of thin films might then be applied to evaluate spatially variable additive manufacturing samples.
- There is a need for in situ methods to observe test coupons during evaluation to provide mechanistic insights. Characterization techniques to interrogate buried interfaces would be beneficial.
- Further development of high-speed and high-resolution field imaging would greatly accelerate insight to transient events.

5. Question 2a: What Are the Key Challenges and Barriers that Must Be Overcome to Apply ML Toolsets for Discovery of New Materials for Application in Dynamic (Impact, Thermal, and Ablative) Environments?

Application of ML toolsets is viewed as necessary to achieve accelerated discovery of new materials for application in dynamic (impact, thermal, and ablative) environments. ML toolsets and software exist but need to be adapted. Full exploitation of the ML approach will certainly require extension and further development to focus on proof-of-concept for material classes of interest in ballistic application. This could be achieved within a generalized and scalable framework that supports rapid, robust, and trusted data exchange. New tools to consolidate data and improved HT workflow will require specialized approaches to transient phenomena (e.g., shocks, heating, localized deformation, and failure). ML models that incorporate these phenomena will rely on physics-based models that target critical mechanisms. Critical (targeted by ML approaches) physics models may require further development. ML offers opportunity to consolidate much of these physics into fast-running analytic frameworks compatible with the HT approach and may be used to guide autonomous systems for HT characterization of transient phenomena.

5.1 Challenges/Gaps

- ML tools for materials science are only just emerging; they currently lack connection to highly specialized physics-based models. Physics-based techniques for ICME are still under development. Scale bridging—quantification of nonlinear bulk properties based on collective behavior of small defects—remains challenging. Direct incorporation of ICME tools within an ML framework could be computationally overwhelming.
- ML-enhanced models for transient phenomenon such as failure are inherently at a disadvantage because the phenomena time/length scale is much smaller than the material/structure scale.
- Current models are not user-friendly; more flexibility is required and models need to account for failure anywhere in the process. To be compatible with ML processes, models need to be reconfigurable as data quality and quantity improve.
- HT methods have varying maturity based on material class. Gaps in the optimization workflow are tightly connected to use-case, which must be carefully considered prior to program initiation.
- Moving voluminous data across platforms is a major challenge.
- Data quantity to train ML methods. Quantity of high-rate characterization is small. Experiments requires care and precision; currently a low-volume activity.
- Data formats are nonstandard and noncentralized. Human inertia is high.
- Uncertainty pervades both bulk materials and final application; quantification is difficult.
- Some ML cannot be easily explained, and can even be difficult to interpret. Information security surrounding ballistic application may impede open across-the-enterprise transparency and only exasperate these issues.

5.2 Potential Approaches

- Apply existing ML codes. Focus on ballistics. Implement ML to facilitate transition between different datasets, serving as “connective tissue” to pass parameters across length and time scales.

- Incorporate better analytic models. Use ML to suggest better analytic descriptors of material properties and link properties to material failure.
- Develop fast models as screening tools. Develop physics-based and ML-based property predictors to identify new composition and processes. Improve computation efficiency.
- Rely on predictive (physics-based) models to improve efficiency of characterization experiments and drive definition of critical data.
- Focus on a centralized data system. Develop upfront plan for secure and agile data exchange—automated processes to move data. Consider if moving data to model or running model on data platforms is most efficient. Data decisions are needed upfront for distributed collaboration model.
- Models or characterization tools that can capture in situ ballistic/high-strain-rate events as well as the pre- and post-event states would allow considerable improvement of some ML-driven models.
- Develop approaches to consolidate data. Develop novel methods to enable inversion of complex experiments with spatial variation at scale to probe failure properties. These methods have been demonstrated for low-strain-rate boundary-value problems but need to be expanded to dynamic problems. A big-data approach to connecting state variables with high resolution will be enabled by ML.
- ML augmented by models can help take the human out of the loop. Develop automation but consider methods to guarantee data quality.
- Use ballistic mechanisms as optimization goal; augment with physics simulation; exploit ML as accelerator.

6. Question 2b: How Will Emerging Machine Learning Capabilities Be Integrated with Emerging Multi-Scale Models, High-Throughput Synthesis, and Characterization to Complete Material Discovery Loops? What Are Key Barriers that Must Be Addressed?

Autonomous decision making is critical to successful implementation of closed-loop material discovery. The appropriate development and integration of machine-directed decision making depends on defining input and expectations of output for each stage of the enterprise. Stages may comprise material synthesis, processing, and/or characterization, and models to connect and inform these stages but will necessarily require HT of information. Machine learning may be considered as a central guiding system or locally guiding (within any one stage) system or for extracting information from individual stages to iteratively direct additional actions. How ML is employed can depend significantly on the nature of data output and maturity of tools, which can differ substantially across the enterprise and be challenged by low-volume or sparse data. Active learning schemes and the like are expected to be important to guide the iterative research loop. There are advantages and challenges with integrating ML in every stage. In the near term, it should be expected that successful loops will be specialized toward narrow tasks. Accumulation of knowledge and experience will support development of more-generalized or modular loops, which may be accelerated by designing modularity directly into research processes, allowing for more-rapid creation of new loops using matured sub-elements.

6.1 Challenges/Gaps

- Sparse data is suboptimal. ML often works best on large data sets, requiring HT synthesis.
- Opportunities for HT synthesis will vary across different materials.
- Moving data between platforms will be challenged by network capability and volume of data.
- Must overcome the language barrier between material science, data science, and automation—as well as between humans and machines.
- Uncertainty management across scales and techniques will be critical.
- Applicability of existing codes, information technology infrastructure–connectivity–collaboration tools, ML tools appropriately optimized, and small data sets that are uncertain.

- ML approaches to high-rate mechanics are not developed.

6.2 Potential Approaches

- Heterogeneous integration of ML capabilities through the design loop, for maximizing value of the data and converting it to information for rapid screening and decision making by the outer loop.
- Integration of ML with ICME toolsets to facilitate scale bridging: Identify key parameters and pass them between models. Identify necessary parameters, and use active learning to drive development of relationships. Establish and preserve relationships and correlations across different datasets.
- Integration of ML to improve guidance of synthesis and processing.
- Integration of ML to improve efficiency of characterization and use as screening tool.
- Physics-based property predictor and/or ML-based predictor to identify new materials and processes. Improve efficiency of calculations and computational cost optimization.
- Use of ML to exploit existing data to find areas of valuable research that have been overlooked.
- Moving data from point A to point B must be part of the up-front plan, where ML analysis may be performed on a different platform than the experiment.
- There are a variety of ML tools already available that may provide a low-risk initial approach, but their application to high-rate mechanics is nascent. Early-term efforts may focus these on transient phenomena (e.g., shocks and localized failure).
- Develop novel physics-based ML tools specific to our application in conjunction with experts in their respective fields.
- Common-language approaches that span disciplines and human–machine interface.

7. Question 3: What Collaborative Models Will Best Increase the Pace of Innovation? How Best to Leverage Resources and Expertise across this Enterprise? Consider Opportunities for Workflow to Discover Materials with Leap-Ahead Performance in Ballistic Applications

A robust collaborative mechanism among government laboratories, academia, and industry is crucial to leverage investments made by the different organizations, accelerate the discovery of new materials, and transition them to the Warfighter. To advance the design timeline, any collaborative research effort will involve many researchers who must efficiently communicate with each other across multiple disciplines and institutions. There are multiple approaches to vertical integration within the collaboration, from having one academic institution lead other academic institutions within the research effort, to having government agencies distribute effort tasks to individual institutions or centers of institutions. Each organizational scheme has advantages and disadvantages that must be considered for any future research effort.

Ideally, a future research effort will involve industry from the start of the discovery process and also take measures to ensure focus while preventing duplication of work. The need to adapt workflow to accommodate evolving HT techniques, desired material classes, and application-specific requirements should be considered in the collaborative structure. These high-risk research goals also carry the task of developing a trained workforce to supply the government labs and industry, so programmatic steps must be taken to bolster this effort as well.

7.1 Challenges/Gaps

- Equipment requirements to accelerate discovery of materials germane to Army applications will be extensive. In some cases, research partners may not know of equipment availability at partner institutions, leading to duplication of spending and development. Survey and communicate capabilities across the collaboration enterprise.
- In the case of a centralized collaboration structure, moving specialized equipment and materials can be difficult.
- Isolating researchers by expertise slows communication and collaboration.
- Bench-level scientists and researchers are often unaware of whom to collaborate with at the start of research programs, especially among institutions.

- Industry rarely sees producing materials and systems for extreme environments as a high-margin endeavor, so they are often not excited to pursue these goals.
- To have multidisciplinary teams collaborate, teams must be able to share data and understand the context of that data. Data generation is typically isolated without a robust mechanism for sharing.
- Legacy collaborative alliances have disposed of useful data and knowledge that could have enriched future efforts or solved problems outside the scope of the alliance effort. Failures and lessons learned are not typically published.
- Engineers and students drawn to ML-augmented methods often pursue opportunities in industries external to the Army.
- The pipeline for talent from academia to industry and government labs is limited to a handful of nonspecific scholarship programs (National Defense Science and Engineering Graduate Program and the Science, Mathematics, and Research for Transformation Defense Scholarship Program).
- Foreign-national students have limited means to join government labs and industry after research programs conclude.

7.2 Potential Approaches

- Award funding levels must reflect the transformational goals of accelerated discovery such that research alliance partners can procure equipment and staff to make these novel breakthroughs.
- Three models of high-throughput integration/workflow were identified:
  - Distributed: centers of excellence with compatible sample and data formats. Advantages: centers are individually accountable to the government agencies for meeting their goals; flexibility of workflow; and capitalize on existing national expertise. Disadvantages: data management is challenging; and sample, equipment, and general collaboration transfer among centers is difficult.
  - Centralized facility: under one roof. Advantages: flexible to workflow changes, and amenable to tiered screening. Disadvantages: resource-intensive, and does not take advantage of distributed expertise.
  - Robot-integrated: automated synthesis to characterization cycle. Advantages: enables greatest integration with AI, and data management

and control software are more easily synchronized. Disadvantages: modifications are challenging; it may not be feasible to integrate with all discovery tasks; and is currently considered a high-risk approach.

- Decentralizing the research effort into centers enables capitalization of expertise at separate locations, but will also require close communication to connect individual centers and avoid duplication of work. Each center could consist of five to seven research leads (e.g., Multidisciplinary University Research Initiative model).
- Offer concurrent small-scale "seedling" awards for smaller teams targeting focused subsets within integrative tasks.
- Build-in mechanisms to ensure regular project turnover to ensure influx of new ideas.
- Hold regular multi-disciplinary and multi-institutional engagements to ensure all partners in a decentralized research alliance structure are kept apprised of each other's efforts.
- Teams must be multi-disciplinary, perhaps going so far as to develop alliance teams with researchers from different disciplines sitting together.
- Researchers and scientists within the effort must themselves have a multi-disciplinary background to be able to communicate effectively.
- Appoint a government point-of-contact to select collaboration leaders from within government at the start of the research effort. The collaboration leader would seek out relevant bench-level researchers within government and connect them to the appropriate scientist in academia or industry. These could be coupled with small 1-year grants or pilot proposals to incentivize cross-institutional collaboration.
- Administer frequent conferences, seminars, workshops, and short courses to foster idea-sharing between institutions and researchers. Attendance from the government workforce will bolster integration of breakthroughs from the research effort to the government.
- Government should seek out industry partners early in the research effort and invite industry representation in research centers. Involving acquisition experts early in the effort will also help focus the goals of the research effort toward something that can be transitioned upon conclusion of the program.

- Utilize Small Business Innovation Research and Small Business Technology Transfer mechanisms to engage industry while providing rapid timeframe (3 years) transition goals.

- Identify or develop a mandatory data-sharing platform early in the research effort. This platform must be endorsed and perhaps hosted by the government agency to introduce a “top-down” condition to participation as a method of compliance.

- Prioritize data standardization early in the research program. Context must be attached to data as well (ensure data conforms to FAIR [Findable, Accessible, Interoperable, Reusable] standards). The government agencies must also conform to the standardization protocol so academic and industry partners have efficient access to government gathered data.

- Standardization of the software and hardware used by researchers can eliminate many of the asymmetries between institutions (i.e., have academic researchers develop numerical models using code platforms that government labs actually use).

- Consider ML- or AI-enhanced methods to extract or organize data when the data is poorly managed to reduce the burden of data organization/standardization on individual researchers. Consider judicious application so as not to burden best practices.

- Research alliance partners must be willing to document and publish failures and lessons learned to draw the full value out of the research effort.

- Government agencies may recruit students for academic research partners as direct hires to the government agency preceding academic enrollment as a student.

- With the aim of developing the government workforce, funding agencies could provide incentives to investigators to retain US-citizen graduate students for their programs. Government agencies could also work with academic research partners to develop recognition incentives for top-performing students within the research program. Recognition incentives might be formalized plans for publications/citations, monetary awards, and so on.

- Government agencies could interface with the existing scholarship programs to advertise placement within their agency upon graduation as a draw to top students.

- Government agencies should offer fellowships and internships to students within the research alliance as a trial for employment.
- Consider opportunities for graduating students and postdocs to continue work on their science as they progress, matriculated to government agencies. Such practices should improve the chance of transition of breakthroughs to the government agency.

8. References

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Appendix. List of Workshop Attendees

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Benji Maruyama	US Air Force Research Laboratory
Berend Rinderspacher	DEVCOM ARL
Betsy M Rice	DEVCOM ARL
Bradford Davis	DEVCOM ARL
Brandon Conover	Practical Scientific
Brian Barnes	DEVCOM ARL
Brian E Schuster	University of Texas El Paso
Bryan M Love	DEVCOM ARL
Bryce Meredig	Citrine Informatics, Inc
Christopher A Schuh	Massachusetts Institute of Technology
Christopher Haines	DEVCOM ARL
Christopher Hoppel	DEVCOM ARL
Corey Oses	Duke University
Dane Morgan	University of Wisconsin
Daniel P Cole	DEVCOM ARL
Danny O'Brien	DEVCOM ARL
David M Stepp	DEVCOM ARL (Army Research Organization)
Debjoy Mallick	DEVCOM ARL
Donald E. Carlucci	DEVCOM Armaments Center
Ed Byrd	DEVCOM ARL
Efrain Hernandez	DEVCOM ARL
Evan J Reed	Stanford University
Frank Fresconi	DEVCOM ARL
George Em Karniadakis	Brown University
George T (Rusty) Gray III	Los Alamos National Laboratory
Ghatu Subhash	University of Florida
Heidi Maupin	DEVCOM ARL
Ichiro Takeuchi	University of Maryland
Jaafar El-Awady	Johns Hopkins University
James A Warren	National Institute of Standards and Technology
James F Newill	DEVCOM ARL
James U Cazamias	DEVCOM ARL
Jeffrey Lloyd	DEVCOM ARL
Jennifer Ciezak-Jenkins	DEVCOM ARL
Jesse Sherburn	DEVCOM ARL
Jim Snyder	DEVCOM ARL
Joel Stewart	DEVCOM ARL
John Clayton	DEVCOM ARL
John Gregoire	California Institute of Technology
John K Brennan	DEVCOM ARL

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Katie Sebeck	DEVCOM ARL
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List of Symbols, Abbreviations, and Acronyms

AI	artificial Intelligence
AMS	U.S. Army Modernization Strategy
FAIR	Findable, Accessible, Interoperable, Reusable
HT	high-throughput
ICME	Integrated Computational Materials Engineering
ML	machine learning
R&D	research and development

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