The Computational Mechanics Vision Workshop

Acknowledgements

The Computational Mechanics Vision and Future Challenges Workshop, which was sponsored by the National Science Foundation (CMMI #1932298, Program Manager: Siddiq Qidwai), was held in Ann Arbor, Michigan on October 31 and November 1, 2019. This final report reflects the contribution of more than 50 technical experts from academia and government. An organizing team of four experts spent several months planning the workshop to ensure focused and productive discussions, while identifying key open issues that must be resolved to help advance the impact of the computational mechanics community. In addition to the organizers, all participants also examined and provided input to the final report.

We are especially grateful for the support from the Michigan Institute for Computational Discovery and Engineering for hosting the workshop, and for assistance from their staff in ensuring that the conference ran smoothly.

Organizing team/participants

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Executive summary

Computational mechanics (CM) is a diverse field with different methodologies and techniques that underlie the solutions of fundamental problems in a variety of application areas. CM techniques have, over the past 50 years, enabled breakthroughs in fields ranging from materials and structural engineering to electronics and bioengineering, in mathematics and high-performance computing. Because of the constant need for predictive computational modeling in both established and newly emerging research fields, CM will continue to play a key role in many future scientific developments.

An organizing team of four[1] experts was assembled to develop a workshop that included more than 50 participants from the CM community, who gathered for a 1.5-day workshop in Ann Arbor, Michigan on October 31 and November 1, 2019. The workshop objective was to solicit and synthesize directions for computational mechanics research and education in the United States over the next decade and beyond.

Four themes were selected for discussion, two vertical and two horizontal. The vertical themes of Machine Learning (ML)/Big Data and Uncertainty Quantification (UQ) and Risk focused on enabling technologies. The horizontal themes of Manufacturing and Medicine focused on application areas. As scientific advances in these emerging areas are coming to the forefront, it is an opportune time for the computational mechanics community to face research and educational challenges and opportunities, and for NSF to make investments to accelerate progress in these areas. Therefore, each of these focus areas was discussed in detail to identify critical gaps and problems that need to be addressed to move the field forward, and to identify other areas where cross-fertilization may be particularly impactful.

In addition to the four thematic areas, which have been organized into subsections labelled Overview, Technical Knowledge Gaps and Emerging Areas of Inquiry, we direct the reader's attention to a short final section on Overarching Themes and Recommendations. Across the four themes the participants expressed the importance of establishing repositories for data, codes and manuals. It was felt that terminology and language remain a hurdle to cross-thematic understanding, and that the establishment of dictionaries would be a notable advance. As new paradigms, such as ML and Risk become more integrated with research, the need for new funding models will become sharper. Finally, continued evolution of CM as a field that builds upon these themes will not be possible without radically new educational initiatives.

We hope that readers will not only find this report informative, but will begin to address the open questions and challenges identified herein. It is clear that computational mechanics has significant potential for enabling transformative breakthroughs in a range of scientific disciplines, and in particular the areas identified in this report.

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[1] Caglar Oskay transitioned to an NSF program director position during the course of workshop organization.

Introduction

CM is a diverse field with different methodologies and techniques that have driven solutions to fundamental engineering problems in a range of application areas. These techniques have, over the past 50 years, enabled breakthroughs in fields ranging from structural engineering to electronics and bioengineering [1]. Studies on the mathematical basis of computational mechanics methods have also driven developments in linear algebra, optimization, functional analysis and tensor calculus. The origins of and advances in high-performance computing are interwoven with developments in computational mechanics. Because of the continuing need for predictive computational modeling in established research fields and the rapidly growing demand for computation in newly emerging fields, CM will play a key role in many future scientific developments. However, although CM has long been central to the developments listed above, it faces new challenges and opportunities from the rise to prominence of artificial intelligence, built infrastructure, additive manufacturing, and an urgent focus on health. This has created a significant need to identify the future challenges and research and educational opportunities facing the CM community in these areas.

There have been several recent NSF-sponsored workshops whose scopes have been relevant and complementary to this meeting. These workshops have focused on verification and validation of computational models [2], and the application of cutting-edge material models and computational algorithms to emerging problems in materials and manufacturing [3].

The current workshop was significantly broader in scope than the recent workshops mentioned above. The focus themes of this workshop, i.e. ML/big data, manufacturing, risk/uncertainty-based engineering (including climate, built infrastructure, natural disasters, etc.), and medicine, have been discussed in other, recent forums. However, as this report details, the discussion in this workshop was not narrowly limited, such as, for instance, to big data in materials and manufacturing. Significant links were also made to problems in medicine, infrastructure, climate change, natural disasters, energy, and other fields. Similarly, while verification and validation is an important and established subfield in CM, it naturally arose within the context of each focus theme we discussed. For this reason, we believe that this workshop will build upon and complement other such meetings, while breaking new ground in many other topics and directions.

This workshop and report were organized to focus on open challenges and opportunities in these focus areas that, if resolved, could enable transformative scientific and engineering breakthroughs. Due to the diverse physical phenomena underpinning the focus areas, as well as the different types of computational approaches that are either currently being deployed or will need to be deployed in the future, workshop participants with a diverse range of backgrounds and disciplinary expertise were invited to participate. Indeed, workshop participants possessed expertise in a wide range of fields, including mechanical, civil, aerospace, biomedical and materials engineering, manufacturing, multiscale and multiphysics modeling, uncertainty quantification, verification and validation, big data, artificial intelligence and high performance computing.

The structure of the workshop is described below. *Internal speakers* presented the view from within the field of CM, while *external speakers* took either a broader perspective, or adopted a specific standpoint from outside what is typically considered to be the current extent of the field.

WORKSHOP PRESENTATIONS

1. Big Data/Machine Learning
    1. Internal speaker: Krishna Garikipati, University of Michigan
    2. External speaker: Nathan Kutz, University of Washington
2. Manufacturing, with a focus on Additive Manufacturing
    1. Internal speaker: Tarek Zohdi, University of California, Berkeley
    2. External speaker: Wayne King, The Barnes Group Advisors
3. Uncertainty Quantification and Risk
    1. Internal speaker: Roger Ghanem, University of Southern California

    2. External speaker: Don Estep, Canadian Statistical Sciences Institute
4. Medicine
    1. Internal speaker: Ellen Kuhl, Stanford University
    2. External speaker: Gerard Ateshian, Columbia University

The workshop began with eight presentations, with two speakers in each of the four focus areas, as enumerated above. For each focus area, a speaker internal to the CM community first spoke to summarize ongoing efforts within the CM community, as well as a discussion of outstanding challenges. Afterwards, an external speaker presented a different perspective on existing needs, challenges and opportunities. The talks were structured in this fashion to entertain differing viewpoints on each focus area, and there were open discussions after each presentation amongst all workshop participants.

After the above sessions organized around presentations, the workshop participants broke into four groups for focused discussion on each focus area. Participants were provided discussion questions in advance, which were common to each focus area. These questions were: (1) What are the areas of inquiry in this space that are currently being investigated by the CM community? Areas of inquiry could be fundamental methodologies or fundamental questions. (2) Which of these areas of inquiry are important but receiving relatively little support? (3) What areas of inquiry do you see emerging in this theme over the next 5-10 years? (4) What are some of the connections between these emerging areas and fundamental questions in the mechanics of materials?

After ample discussion time (four hours spread over two days) by each breakout group, all workshop participants reconvened to discuss the findings and recommendations of each group. The recommendations and findings of each breakout group, augmented by the subsequent discussion amongst all participants, forms the basis for the recommendations for future research presented next.

Summary of Focus Areas

Machine Learning

1: Overview

Machine Learning (ML) has a rather natural relevance to computational mechanics. Broadly, this connection comes into play for handling deluges of data--whether these data are to inform computational mechanics, or are produced by it. In the first scenario, machine learning approaches can describe phenomena in complex systems where we do not yet have a good physical understanding. In the second scenario, it can provide new and efficient tools and frameworks to organize and interpret large scale computed data.

The CM community has already begun using ML for a variety of applications. Some of the most prominent are: (1) Modeling constitutive and phenomenological relationships. While the development of experimentally-guided models has been central to mechanics, the volume and complexity of data used for this purpose has heretofore been rather modest. From neural networks to Gaussian processes, and with techniques stretching from active to reinforcement learning, the bridge between experimental data and constitutive models can now be built with previously unapproachable sophistication. (2) Discovering governing physics (i.e. PDEs) or for system identification. This is one of the most compelling fronts unifying ML and CM. Inverse modeling already incorporates the field of system identification: the pinpointing of physical mechanisms, or even entire systems of PDEs that govern spatially and temporally varying data. The holy grail in this regard is the discovery from data of physics (perhaps as PDEs) that was previously unknown. (3) Accelerating solutions to PDEs via physics-constrained/informed ML. Here, the CM community has been solving initial and boundary value problems with ML methods that circumvent traditional numerical techniques such as the finite element method. Now, ML methods, from neural networks of all types to genetic algorithms and Gaussian processes, present the possibility of learning solutions to PDEs. In particular, work has focused on accelerating solutions via surrogate models that replace expensive, high-fidelity simulations in prescribed regimes of parameters and domains.

2: Technical Knowledge Gaps

A key challenge is in analyzing and characterizing different ML methods. For example, what are the tradeoffs among different ML approaches, and what are the guidelines to choosing the correct one? How reliable and robust are the ML solutions, and what are the convergence rates for different ML methods? What are the error bounds for ML solutions, and can we quantify the uncertainty in the solutions?

There are also issues related to understanding interpretability, predictability, and generality of ML models in CM, which is important for connecting the results and performance of ML models with physics, or for embedding known physics into ML. Furthermore, ML networks are very good at data interpolation, but it is less clear whether they are capable of extrapolating to out-of-training regimes or when data are sparse. This may be particularly relevant for characterizing failure using ML (which may necessitate involvement of UQ and risk analysis), particularly since failure points often have sparse data to train an ML model. Overall, challenges and opportunities remain regarding the ability to gain scientific insight and discovery using ML.

The issue of using ML for scale-bridging, i.e. to detect and capture features at different scales, or to use ML to decouple physics at different length and/or time scales, is a key challenge. There are also opportunities in using the ML modeling error to adaptively redesign the ML architecture using physics-based knowledge to improve the property predictions. Overall, there is a pressing need to integrate ML, physics-based modeling and experiments, and a workflow for closing the loop among them (i.e. the design of high-throughput experiments for supporting ML). Finally, there are natural but unexplored links between UQ for ML and ML for UQ. This tight integration between ML and UQ would support inverse problems while preventing overfitting and enabling the treatment of noisy and sparse data regimes. This is crucial for risk and failure analysis.

Another challenge relates to data sharing and the creation of challenge and/or benchmark application problems for the CM community. In particular, it is important to ensure diversity of benchmark problems of different sizes, with good coverage of the application space, and of relevance to both research and student education. These benchmarks should also include a range of metrics for comparing various ML methods beyond just accuracy (e.g. uncertainty, robustness, reliability, speed, etc.). This would enable and grow the contribution of the CM community, while promoting these sharing platforms and challenge problems at conferences and with neighboring communities (e.g. applied math).

3: Emerging Areas of Inquiry

Over the next 5-10 years, we foresee the emergence (or growth) of the following main themes under ML in CM: (1) The acceleration of solutions to PDEs; (2) the emergence of AI in manufacturing (i.e. smart manufacturing); (3) the emergence of ML in mechano-biology; (4) the emergence of ML in bridging physics across disparate length and time scales; (5) the integration of ML, physics-based modeling, and experiments.

With regards to the intersection of ML and fundamental questions in mechanics, we foresee the emergence (or growth) of the following main themes: (1) The ability to predict material or structural behavior under extreme conditions. The complexity of failure with multiscale and multiphysics processes presents opportunities for application of a range of ML frameworks and specific techniques. A challenge in this regard is the sparsity of data around failure events, and the challenge of acquiring more data. (2) The ability to predict stochastic phenomena. Turbulence is a leading example in this regard, and one in which ML methods already have made significant inroads. (3) The ability to rationally design functional materials driven by high-dimensional and complex dependencies. (4) Design optimization: High-dimensional optimization problems are particularly well-suited to ML. (5) Prediction of structure-function relationships: The expressiveness of ML methods at representing high-dimensional and complex dependencies is an advantage over other approaches.

Overall, we recommend the following action items to facilitate bringing ML into the CM mainstream: (1) Data sharing and creation of challenge application problems for the community; (2) making research codes available to the public; (3) unifying language and terminology, while building “dictionaries” for terminology from other fields and communities; (4) educating the CM community, while strengthening the themes of statistics and probability in undergraduate and graduate student education.

Medicine

1: Overview

Computational medicine can be defined as physics and data-driven computation applied to gain fundamental understanding in biology/physiology and to patient care (detection, diagnosis and treatment of disease, and prognosis) in medicine. Problems in computational medicine can often be of two very different types.

On one hand, there are problems where the goal is to understand in detail the biology/physiology of a given system. For these problems, there is a plethora of data, the ability to collect data of the type that is believed to be the most relevant, and minimal time restrictions with regards to scientific inquiry. On the other hand, there are problems that emanate from medicine and are of a translational nature, where the goal is to improve a patient’s health outcome. Here, the data is collected in a clinic independently of computational mechanics researchers. This in turn places constraints on the type of models that can be used to solve these problems.

Both of these general types of problems are challenging to solve, and computational mechanics researchers have accordingly realized that a piecemeal approach to solving them does not work. This has led researchers to develop methods and techniques that couple biology and medicine with other fields of computational physics like mechanics, electromagnetics and biochemistry. Researchers have also recognized that these problems are often multiscale in nature, where responses at the cellular, tissue and organ scales all interact with each other and have a critical role to play in the final outcome. Finally, due to the heterogeneous nature of biological systems it is important to infer parameters that are specific to a given subject, organ and tissue. This has led researchers to consider the use and development of techniques of inverse problems in order to infer these parameters.

2: Technical Knowledge Gaps

While some biological systems, such as the cardiovascular system and brain, have (deservedly) received significant attention, other important ones have not. Lung mechanics, the venous system, the reproductive system, and skin are examples of systems that have not received the same type of attention and are ripe for further in-depth studies.

Due to the dramatic recent growth in the number and types of implants that are now routinely used in the human body, there are important questions to be addressed on how implants and devices interact with native tissue. Examples include heart implants interacting with soft tissue, electrodes in the brain, and stent meshes that tear through vasculature.

There are broader issues that connect to all of the open application areas mentioned above. For example, there is an untapped potential in formulating studies that utilize the data already collected in studies sponsored by agencies like the NIH. Furthermore, imaging, which is fundamental to diagnosis and insights into biological systems, contain a wealth of physical data. It will be of interest to formulate studies that can use medical images, which are obtained through elastography and contrast enhanced imaging, to infer the physics of biomedical systems. This also demonstrates the importance of conducting scientific studies where computational modeling and experiments are tightly linked.

Finally, there is a need to develop curated data sets for benchmarks and validation. These could be general or organ-specific. This could be an area for separate investigation and discussion through another workshop, while noting that the ML community in particular has very effectively developed such benchmarks in fields such as plasticity and fracture mechanics.

3: Emerging Areas of Inquiry

Some of the emerging growth in computational medicine dovetails with some of the other workshop themes, in particular ML and UQ/risk. ML will intersect with computational medicine because the complexity of phenomena in medicine and biology is such that it is almost impossible to develop predictive physics-based models for every problem of interest. Thus, one has to rely on a combination of data and physics-driven models. Risk will intersect with computational medicine because the decisions made in computational medicine can have a profound impact (Is a given tumor is cancerous? Will a given treatment be effective? What is the underlying cause for a disease? Etc.). Thus, it becomes necessary to quantify uncertainty or risk in any prediction.

In addition to these intersectional themes, broad challenges were identified. (1) Is it possible to map from animal or lab-on-chip models to humans? This is a challenging problem, but one with a tremendous potential payoff, as it shares features with the fields of transfer learning and domain adaptation in machine learning. (2) How can modeling across the disparate biological timescales be achieved? Molecular time scales are $\sim 10^{-9}$ s and cellular time scales are $\sim 10^{0}$ s, while aging happens on timescales of $\sim 10^{9}$ s, thus implying a total range $\sim 10^{18}$. While it is recognized that most problems in biology and medicine span multiple spatial scales, not much attention is paid to this tremendous range of temporal scales. (3) The study of emergent properties: mathematically, these appear as bifurcation problems. For example, a small perturbation during cell division leading to organ buckling. (4) Inferring fields and system behavior: while current research has focused on inferring parameters, future trends point to inferring entire biophysical fields and systems from measurements. (5) The problem of computational drug delivery and efficacy improvement, where surface properties at the nanoscale are manipulated to design more effective drugs. (6) Finally, optimization at larger scales to achieve bioprinting and design of tissue with desired properties is of growing interest.

The themes discussed in the previous paragraph include research in some fundamental areas of applied, theoretical and computational mechanics. These include the problems of growth, remodeling and aging and fracture/fatigue in biological environments. One very interesting approach aims to use synthetic biology as a deconstructionist tool to study mechanics. Broadly speaking, this involves using tools of synthetic biology to design systems where one can isolate effects and answer some fundamental questions related to biology and medicine. In addition, mechanics coupled with other physics (so-called coupled-field or multiphysics phenomenon) still has a long way to go in terms of modeling biological systems. Finally, along the same lines, there are many interesting biological processes, like thrombosis, cell migration, morphogenesis, for which continuum mechanics-based models are still in their infancy, and better and more useful models are required.

Additive Manufacturing

1: Overview

Computational mechanics research of relevance to additive manufacturing (AM) can be classified into five areas: (1) Process modeling; (2) product performance modeling; (3) design and optimization of the manufacturing process or the product performance; (4) preprocessing – modeling of how the constituent material (e.g. powder) is processed; (5) postprocessing – modeling of recrystallization, hipping, sintering, etc. to achieve better or more uniform performance. While AM is a highly researched area, it is estimated that less than 10% of AM literature is on modeling and simulation[2]. The physics of AM processes and the possible design spaces enabled by AM have become hugely complex and the lack of fundamental, computationally-driven research has prevented AM from being fully adopted today.

Reviewing the state of the art literature today, there is active research in studying the microstructures (e.g. grain structure, porosity/void evolution, grain remodeling, dendrites, and secondary phases) and their modeling to predict material performance. In the context of mechanics and modeling of AM processing, the majority of literature has been dedicated to the thermal residual stresses and distortion although the current capability cannot yet predict thermal stress or strain. The second common area of investigation is in process modeling such as modeling the melt pool, energy source and phase transformation. While some of the pre-AM research in material thermal physics and welding provides useful information to AM processing, there are AM-specific issues that the focused efforts have not resolved. Figure 1 summarizes the current literature survey results on AM modeling and simulation.

Another area of active research discussed is topology optimization (TO). Topology optimization has been developed and researched independent of AM and the current areas of interest are in the design of coupled physics and coupled scale problems. Of course, the topologically optimum designs can be manufactured using traditional manufacturing techniques. However, TO has been identified as an ideal design method that can maximally exploit the flexibility of AM. The recent rise of multiscale topology optimization is said to have been motivated by AM which can manufacture a wide range of scales without significantly added complexities. Much of TO research, however, is somewhat independent of AM and research in TO specifically for AM accounts only for a small proportion of TO research. There are many outstanding AM design challenges.

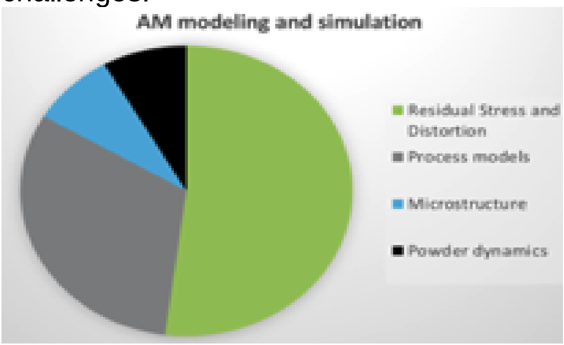

Figure 1. Literature survey of AM modeling and simulation[2], © The Barnes Group Advisors LLC

[2] King W.E. (2019) "Computational mechanics and additive manufacturing as seen from the outside of the core computational mechanics community", presented at NSF Computational Mechanics Workshop, Ann Arbor MI.

2: Technical Knowledge Gaps

The current state of computational mechanics in AM is that there is substantial funding and activities in the commercial sector to adopt AM in production. These are primarily seen in industrial and government funded activities and the rapid emergence of AM related software. However, there is a lack of fundamental understanding and basic research, leading the current state of the art software to be unpredictable and unreliable, using the empirical and experimental data at best. Therefore, all areas of inquiry in fundamental sciences at a basic research level are currently receiving little or no support, and is in great need to be supported to move forward AM in practice.

For each of the five specific classes of AM related computational mechanics research, the areas which require further inquiry are identified below.

For process modeling: (1) Residual stress and distortion, sag modeling; (2) thermal modeling (multiphysics); (3) microstructure models (grain structure, porosity/void evolution, grain remodeling, dendrites, and secondary phases, etc.); (4) powder dynamics and slurry dynamics including delivery systems; (5) repeatability and reproducibility; (6) melt pool, energy source, optical, phase transformation modeling; (7) material-interface modeling; (8) development of process models that are able to bridge length and time scales present in metal AM; (9) process models that can predict defects in the AM build.

For performance: (1) Microstructure to performance modeling; (2) in-situ NDE and real time optimization of manufacturing parameters; (3) multiscale methodologies to address lack of scale separation (for homogenization) in AM.

For design and optimization: (1) Process aware TO and its integration in the overall CAD design; (2) top down systems approach to design of integrated material-structural systems; (3) avoiding and/or optimizing for support structures; (4) functionally graded materials and multiple materials;

(5) mesostructure design (architected materials); (6) design and control of microstructures (grain level); (7) AM specific uncertainty quantification and risk in optimization; (8) digital threads;

For preprocessing: (1) modeling of powder processing; (2) supply chain

For postprocessing: modeling of (1) recrystallization; (2) hipping; (3) sintering.

Of this long list of topics, the following areas have been identified as receiving minimal support: (1) Performance prediction from complex multiscale multiphysics modeling. The level of complexities is such that the current computational cost is prohibitively high for practical applications. (2) Processing modeling including melt pool, energy source, optical and phase transformation modeling; (3) topology and multiscale optimization.

3: Emerging Areas of Inquiry

There is a significant need for fundamental research to predict material properties and performance, which is not addressed by existing applied research. The challenges are highly complex requiring an integrated and coupled modeling of nonlinearity, solid and fluid mechanics as well as powder and slurry dynamics and phase transformation. The current state of the art in high-fidelity modeling is computationally extremely demanding and limits its application and practical use.

The current state of the art is also not capable of predictive modeling and this inherently limits AM's application, especially in safety critical engineering. For AM to be fully exploited in engineering, a predictive modeling capability is critically important, but it is currently limited by the lack of fundamental understanding. The complexity of the challenges is such that it requires collaborative and integrated multidisciplinary team approaches. It would benefit from establishment of an open research platform (software, hardware and databases) that enables cooperative research and a common ground for building up the complexity. The appropriate use of modern methods such as artificial intelligence and ML may provide useful means to manage the complexity of the AM process, for example in detecting defects and understanding the residual stress in the initial state.

In order to fully utilize AM, a design optimization method is needed. Here, topology optimization is considered the ideal design method. Such physics-based design methods require reliable computational methods which can reliably and robustly offer accurate and stable sensitivity analysis in a computationally efficient and repeatable manner. Given the inherent uncertainties associated with AM processing, research is needed to develop topology and design optimization methods that can account for the uncertainties and mitigate the risks. In addition, AM presents new challenges in terms of manufacturing constraints and requirements. More attention is required in design optimization research such that the design process and method are aware of each other.

In addition to these challenges, there are several important directions that emerged connecting CM, AM and mechanics of materials:

(1)Rethinking multiscaling of mateials and structures in the context of AM. AM inherently integrates material processing and structural design. These two concepts cross unprecedented length and time scales, and computational mechanics and design optimization are needed to integrate the understanding of scales as well as multiple physics and multiple materials. This

introduces a new paradigm shift in design – towards an integrated material-structural system. This departs from the traditional design philosophy of decoupling material processing and structural design, where material design and processing and structural designs are done in a serial way. AM requires an integrated understanding of these traditionally separate disciplines and will require new paradigms to integrate materials and structural designs. The complexity of such multiscale mechanics also means that providing the forward tools and relying on human intuition to understand and design is no longer sufficient. These complex multiscale behaviors go beyond intuitive understanding. Research is needed to develop design optimization methods based on computational mechanics and forward models in order to fully explore the hugely expanded and complex design spaces.

(2) *Real-time monitoring and process redesign*. CM is needed to support on-line monitoring and in-situ non-destructive evaluation (NDE) to assess the design and determine the optimum process. In-situ NDE for AM is underway, but without fundamental understanding of the mechanics and processing, it is unclear how best to utilize the data to affect the processing. This kind of computation also requires new and innovative computing tools that can provide real-time understanding to redesign the processing parameters such that the final part meets the requirements.

(3) *New perspectives on voids/defects (defect minimization and mitigation)*. The creation of voids is an inherent part of AM and can degrade material performance. Research efforts have thus been focused on minimizing and eliminating voids hence reducing the property variations. However, a different perspective is that the voids (what are traditionally considered defects) are unavoidable. With this new perspective, future research can shift to predicting and managing the voids, reducing the material property variations, design in the property variations where they matter, and designing against the uncertainties introduced by the voids. This new set of computational mechanics approaches can widen the applications of AM.

While many possible paths forward are presented here, the importance of integrated experimental and computational research should not be understated. This naturally incorporates UQ and verification and validation, which is pertinent given the complex challenges AM presents. Furthermore, this implies that future CM research in AM would benefit from a team-centric approach, which is also a requirement to enable the fundamental understanding of the coupled multidisciplinary and multiscale nature of AM processing. Therefore, successful research to gain fundamental scientific understandings of CM in AM in the future would need to engage multiple investigator teams integrating multidisciplinary experts.

Finally, it is important to note the democratization of manufacturing that AM has enabled. While the above discussion makes clear the unprecedented scale of scientific challenges in the field, and somewhat cautions against currently employing AM in practical engineering design, there are already growing internet communities that share free topology optimization software, AM STL model file repository sites and YouTube videos on how to optimize and achieve the best designs. AM coupled with TO is likely to have a large societal impact. Computational modeling to understand the societal impact and potential risks to the society may thus prove to be beneficial. This requires multidisciplinary research with social sciences and/or humanities, and is aligned with two of the NSF's 10 big ideas: Future of Work at the Human-Technology Frontier and Growing Convergence.

UQ/Risk

1: Overview

Uncertainty quantification (UQ), once an emerging area of computational science, has now become a fundamental underpinning of computational mechanics. A broad range of topics within UQ has therefore been or is currently being investigated, covering probabilistic modeling (How can one represent random input quantities?), uncertainty propagation (How can one accurately and efficiently propagate random inputs through a model?), and identification (How can one calibrate a set of model- and hyper-parameters, based on some digital or physical observables?) and validation aspects (How can one assess the relevance of the aforementioned strategies?).

2: Technical Knowledge Gaps

From a stochastic modeling perspective, the integration of constraints (such as boundary conditions, or symmetries) in stochastic reduced-order models and surrogates, together with the treatment of non-stationary, non-Gaussian models, are needed to advance physics-based UQ. While the design of robust stochastic solvers (including, e.g., quadrature schemes for collocation methods) and sampling algorithms for high-dimensional (i.e. with many degrees of freedom, and also many random variables) computational models has been a very active research area over the past decade, efforts are still required to attack realistic problems that combine multi-physics information across scales and (space and time) domains. For UQ to achieve further adoption beyond academic studies, these efforts should be supplemented with the development of appropriate error bound definitions that are scalable to large-scale applications.

Moreover, the development of UQ strategies adapted to rare events (in terms of modeling, sampling, and data integration) is necessary to enhance current practice in risk analysis and related fields (such as decision making under uncertainty). Finally, there is an absence of standards regarding benchmark validation, reproducibility, and more generally the definition of "well-posed" UQ problems, which is compounded by limited knowledge and skills on core topics such as data science, statistics, and uncertainty quantification. The latter aspect points to the need for new curricular considerations at the undergraduate and graduate levels, while simultaneously making the field-specific language more accessible for non-specialists.

3: Emerging Areas of Inquiry

The robust treatment of *model* uncertainties (as opposed to *parametric* uncertainties, which are traditionally introduced to model variability in the parameters of the computational model) and data-driven, UQ-based physics and structure discovery are seen as two emerging topics in stochastic modeling. Example application areas for model uncertainties are closure for flow problems, and the uncertainties introduced by different types of interatomic potentials in molecular dynamics simulations, while an emerging example for structure discovery concerns the identification of constitutive models based on limited data. In addition, the proper treatment of non-stationary, non-Gaussian fields will be necessary to perform uncertainty quantification in multi-scale systems, for example in materials processing in additive manufacturing applications.

There are important challenges to resolve in data assimilation, where there is a need to develop integrated frameworks and methodologies to integrate physical experiments within UQ frameworks, for example in the context of Bayesian approaches or probabilistic learning. In this context, the treatment of partially observed systems (for example a 3D system characterized by 2D measurements as in the case of digital image correlation) remains a challenging problem for which robust methodologies for identification and updating have to be developed. Finally, for UQ to impact industrial applications, a stronger integration of UQ in the engineering workflow and design process, which could be achieved through the development of community software, is essential.

There exist numerous connections between the above challenges, and the potential to tackle fundamental questions in mechanics of materials if they are addressed. First, there is an opportunity to strongly integrate UQ into existing design standards. A second opportunity concerns accounting for uncertainty in model discovery and model error assessment, with specific examples being: (1) model updating, for example through adaptive model selection based on plausibility, (2) the development of predictive models at the material and system levels (in the form of constitutive relations for the former case), (3) the identification of critical variables by means of global sensitivity analyses, (4) the propagation of variability through length and time scales, and (5) modeling for configurations far from equilibrium (e.g., modeling at high strain rates, accounting for geometric and/or material nonlinearity).

Furthermore, in connection with other workshop themes, it was recognized that knowledge in mechanics of materials should be used to derive meaningful constraints for different application areas involving machine learning techniques. Finally, progress in stochastic modeling could lead to enhanced statistical modeling of heterogeneous media and defects, and would enable the solution of problems in which data is obtained through different modeling assumptions (e.g. predictions obtained with different mesh densities).

Finally, it is important to emphasize the NSF GOALI program, especially with respect to the integration of state-of-the-art UQ techniques in workflows. The importance of encouraging interdisciplinary teams with expertise in computational mechanics, materials science, and uncertainty quantification to solve challenging problems in mechanics and other fields, should also be highlighted.

Overarching Themes and Recommendations

Though the discussion groups focused on the four overarching themes (Medicine, UQ/Risk, ML, Manufacturing) of the workshop, several elements arose in all discussions in addition to the specific technical challenges for each area.

A first issue that arose in all focus area discussions is the need to establish field-relevant and field-specific open source repositories that house benchmark data, which is essential for challenge, benchmark and validation problems. These repositories also should contain existing codes along with manuscripts and documentation that can be used to demonstrate reproducibility. Correspondingly, the NSF and other funding agencies should consider long-term support of software maintenance, which is distinct from the current funding model of supporting funding for model and method development. Finally, it is important to incentivize the sharing of codes and data that result from federal funding, to enable the growth and visibility of these open source repositories.

A second issue concerns the fact that as CM becomes a convergent discipline in the sense that it is needed in nearly all emerging and critical scientific disciplines, there is considerable difficulty and confusion that arises from the lack of common language and terminology across disciplines. This confusion hinders or significantly delays researchers from considering these multidisciplinary scientific challenges. The CM community would benefit from such a unification, perhaps through building dictionaries from other fields and communities.

Third, many discussions centered around the need for new funding models that reward truly interdisciplinary teams involving engineers, biologists, mathematicians and statisticians, computer scientists, etc., that are needed to tackle the complex technical challenges that emerged from the workshop. Furthermore, there are opportunities for the NSF and other federal funding agencies, industry and National Labs to formulate and support research challenges and open questions; for example, a common theme between all focus areas was the challenges involved in modeling material fracture and failure. Existing funding possibilities that could enable such projects include NRT or GOALI calls, though it seems likely that new, interdisciplinary funding mechanisms may be most effective in meeting this objective.

Finally, participants recognized the need for new educational paradigms given the current disconnect between current undergraduate and graduate curricula, and the emerging focus areas discussed at the workshop. For example, for ML and UQ/Risk to have better practitioners and users it will require strengthening themes of statistics and probability at all educational levels. Furthermore, the complex, multidisciplinary nature of these problems also points to a need to educate current researchers. Focused tutorial-based workshops that are meant to educate attendees represent one possible approach to help achieve this objective.

REFERENCES

1. “Simulation-Based Engineering Science: Revolutionizing Engineering Science through Simulation”, Report of the NSF Blue Ribbon Panel on Simulation-Based Engineering Science, 2006. Electronic copies available at: https://www.nsf.gov/pubs/reports/sbes_final_report.pdf
2. “Verification & Validation of Computational Models Associated with the Mechanics of Materials”, The Minerals, Metals & Materials Society (TMS), 2018. Electronic copies available at: TMS Verification and Validation
3. “Advanced Computation and Data in Materials and Manufacturing: Core Knowledge Gaps and Opportunities”, The Minerals, Metals & Materials Society (TMS) 2018. Electronic copies available at: TMS Core Knowledge Gaps