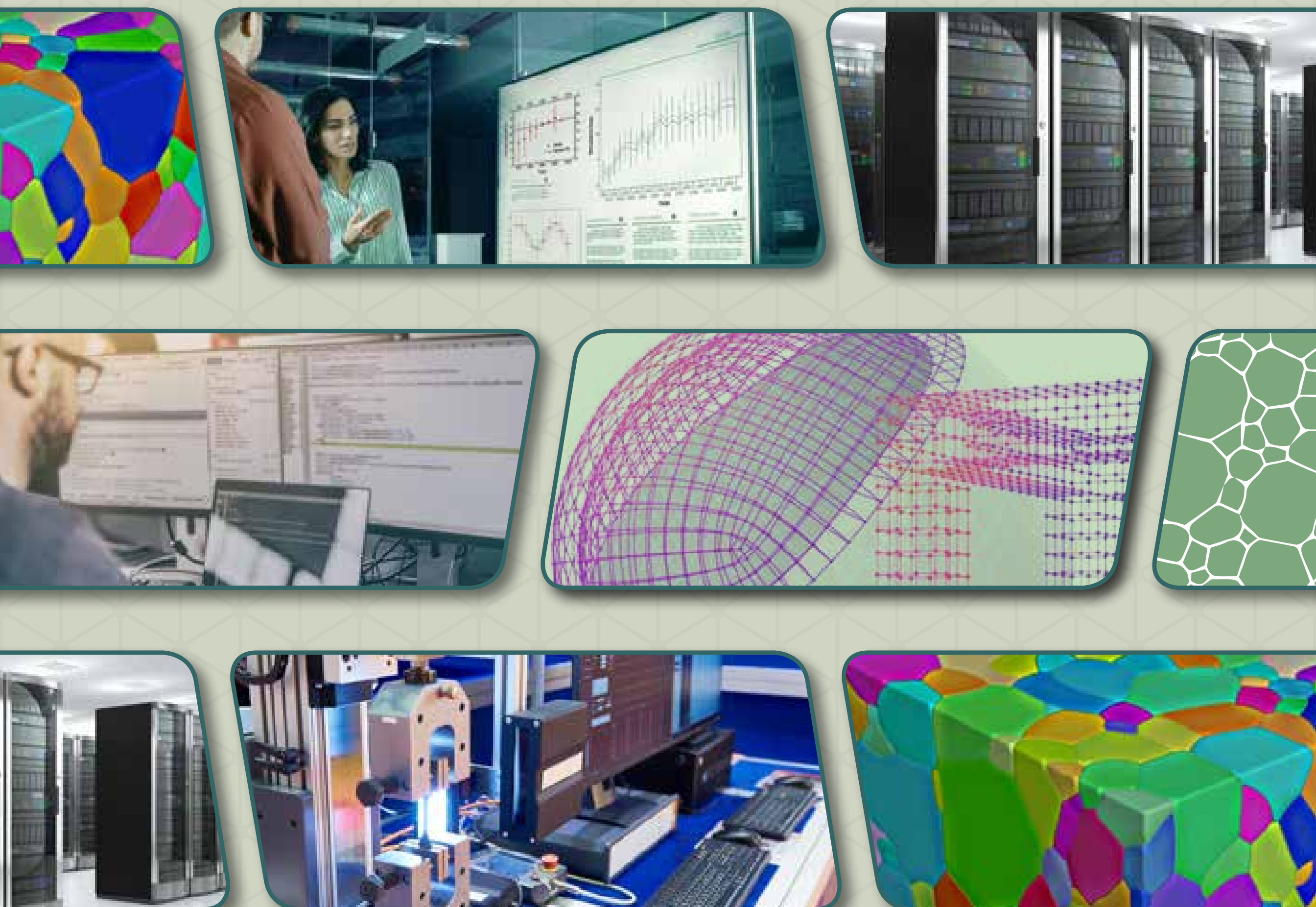
V&V

VERIFICATION & VALIDATION

OF COMPUTATIONAL MODELS ASSOCIATED WITH THE MECHANICS OF MATERIALS



TMS A Study Organized by The Minerals, Metals & Materials Society

Verification & Validation of Computational Models Associated with the Mechanics of Materials

V&V VERIFICATION & VALIDATION

OF COMPUTATIONAL MODELS ASSOCIATED WITH THE MECHANICS OF MATERIALS

A STUDY ORGANIZED BY

The Minerals, Metals & Materials Society (TMS)

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DOI: 10.7449/VandV_1 ISBN: 978-0-578-45369-9

The Minerals, Metals & Materials Society (TMS)

Promoting the global science and engineering professions concerned with minerals, metals, and materials

The Minerals, Metals & Materials Society (TMS) is a member-driven, international organization dedicated to the science and engineering professions concerned with minerals, metals, and materials. TMS includes more than 13,000 professional and student members from more than 70 countries representing industry, government and academia.

The society's technical focus spans a broad range—from minerals processing and primary metals production to basic research and the advanced applications of materials.

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To facilitate global knowledge exchange and networking, TMS organizes meetings; develops continuing education courses; publishes conference proceedings, peer-reviewed journals, and textbooks; leads technology studies and reports; and presents a variety of web resources accessed through www.tms.org.

TMS also represents materials science and engineering professions in the accreditation of educational programs and in the registration of professional engineers across the United States.

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Acknowledgements

The *Verification & Validation of Computational Models Associated with the Mechanics of Materials* workshop and report were executed by The Minerals, Metals & Materials Society on behalf of the National Science Foundation (grant #CMMI-1812449; Program Director - Dr. Siddiq Qidwai). The final report draws on the contributions of 40 internationally recognized technical experts from academia, industry, and government who took part in an interactive, facilitated workshop in New York, New York on July 27, 2018. An organizing team of seven experts spent several months planning the workshop to help ensure productive discussions and informative outcomes that could help to advance the materials and mechanics community in its use of advanced computation and experimental data tools and resources to verify and validate computational models. In addition, a separate review team of experts also examined a final report draft and provided comments.

The dedication and active involvement of the subject matter expert volunteer groups were critical to the success of this effort. We are grateful for their time and contributions and hope that this report helps to inspire individuals, groups, and large organizations to undertake the activities outlined in the document. There is great promise in advanced computation and data-enabled science and engineering, but it is predicated on robust and accurate verification and validation of the computational models, and we are excited by the opportunities it presents for new materials and manufacturing innovations.

Steve WaiChing Sun, *V&V* Organizing Team Chair
George Spanos, *V&V* Project Leader

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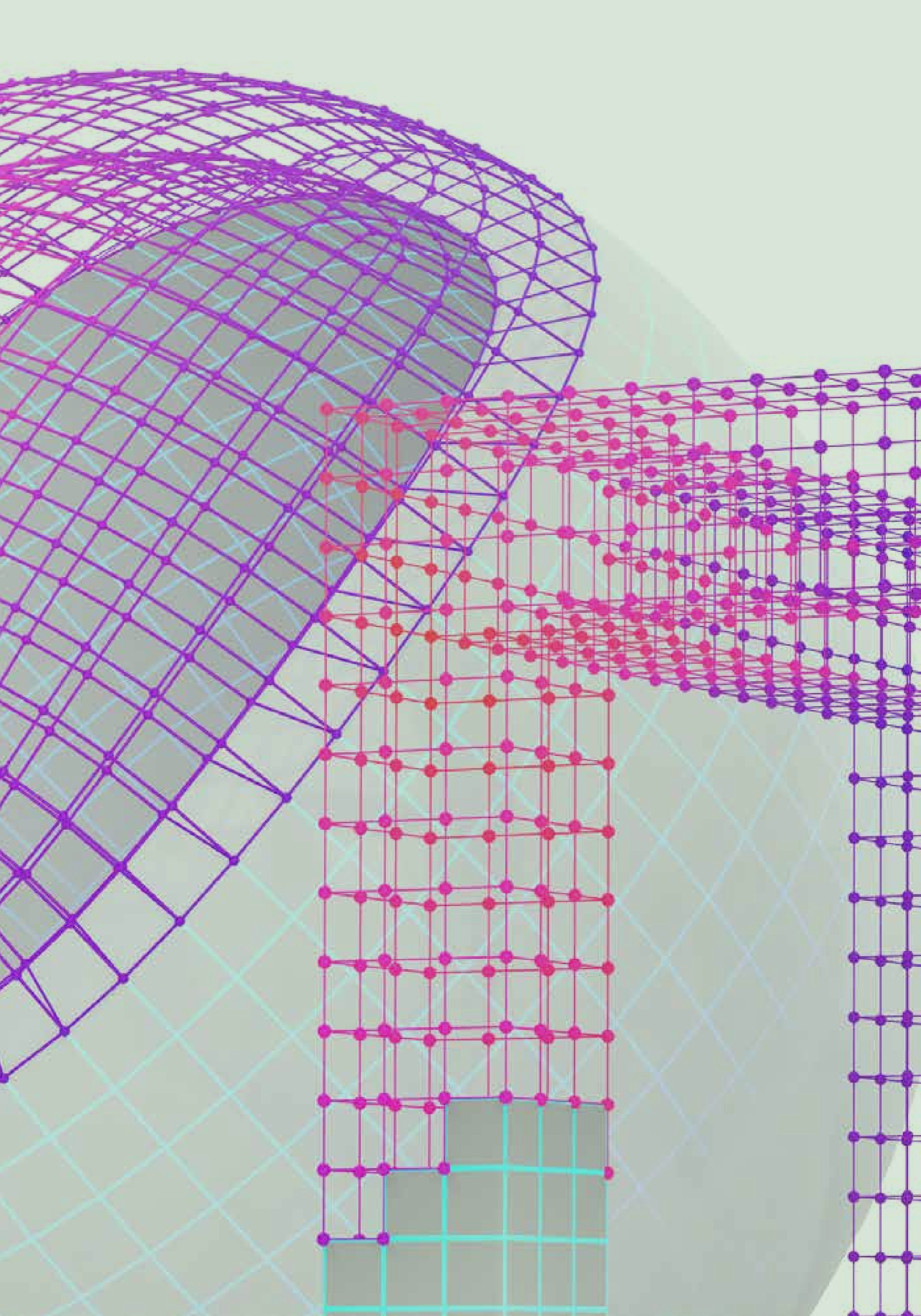
The project leader of this effort was George Spanos, TMS Director of New Initiatives, Science, and Engineering, with strong support from TMS staff members Owen Daly (Technical Communications Specialist), Michael Rawlings (Science and Engineering Lead), and Justin Scott (Technical Project Leader, and Principal Editor of JOM). The volunteer workshop participants listed above provided the detailed study inputs, which were compiled into this final report format through the efforts of TMS staff. In addition, other TMS staff who contributed to the final report include Matt Baker (Content Senior Manager), Maureen Byko (Editor, *JOM*), Bob Demmler (Graphic Designer), David Rasel (Media Manager), Lynne Robinson (Head of Strategic Communications & Outreach), and Marleen Schrader (Accounting and Human Resources Specialist). Nexight Group LLC staff members, who were instrumental in the workshop facilitation and content capture and organization, include Ross Brindle (Chief Executive Officer), Jared Kosters (Technical Project Manager), Jack Holmes (Research Analyst), Rachel Lanspa (Technical Writer and Editor), and Changwon Suh (Senior Technical Consultant).

Preface: Who Should Read This Report

This report contains information of high value to scientists, engineers, and designers within the materials and mechanics communities, and to individuals from a variety of other disciplines spanning the academic, industrial, and government sectors. More specifically, computational, theoretical, and experimental researchers and developers associated with mechanics and materials who utilize advanced computation and data tools should find the information in this report especially valuable. Since much of the content in this report relates to helping shape the future use of advanced computational modeling in the MOM, organizations and individuals who influence the future of such efforts will find this report useful, including those who support financial investments in science and technologies surrounding such predictive computational modeling. Educators teaching undergraduate and graduate courses related to this topic, as well as department heads within the relevant disciplines, could use the information in this report to advance associated curricula and research. Other stakeholders who may find this report useful are decision-makers at federal agencies, including program managers. Likewise, leaders supporting the manufacturing industry, such as the Department of Defense (including ManTech and its other entities that support manufacturing), and the leadership and members of the Manufacturing USA Institutes could use the information in this report to help mold the future of effective computational modeling in manufacturing.



Executive Summary

Background and Motivation

Predictive computational models associated with the mechanics of materials (MOM) offer great potential for enabling large reductions in the cost and time to develop new products and manufacturing procedures. Unfortunately, this potential is currently limited because very rarely are such models adequately and broadly proven to yield trustworthy, accurate, quantitative results for which the level of uncertainty has been quantified. In this regard, the need for rigorous verification and validation (V&V) of these models cannot be overestimated, yet is extremely lacking within the relevant MOM communities. There is thus a strong need to help these communities accelerate the widespread adoption and implementation of such V&V activities.

In this vein, concise definitions of verification and validation have been provided by the American Society of Mechanical Engineers (ASME),[1] and can be applied here as well:

- **Verification:** The process of determining that a computational model accurately represents the underlying mathematical model and its solution
- **Validation:** The process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model

The overarching goal of this workshop and report is thus to help facilitate the widespread and rigorous adoption of V&V by both computational modelers and experimentalists in MOM-related communities.

Workshop and Report Process

The *Verification & Validation of Computational Models Associated with the Mechanics of Materials* workshop and report were executed by The Minerals, Metals & Materials Society (TMS) on behalf of the National Science Foundation. This final study report draws on the contributions of 40 internationally recognized experts from academia, industry, and government, primarily based on their ideas and outputs from an interactive, facilitated workshop held in New York, NY on July 27, 2018, adjacent to the 13th World Congress on Computational Mechanics (WCCM).

Barriers to V&V Adoption

Thirty-one barriers preventing the adoption of robust V&V approaches within the MOM community were identified in order to provide a foundation from which efforts to overcoming these barriers could be developed. Four overarching challenge categories and six barriers representing the largest impediments to widespread V&V adoption were then prioritized and presented in Table III, which is reproduced below. These barriers (discussed in more detail in Section III) were then used as a foundation for helping to develop some overarching opportunities and recommendations (Section IV), as well as detailed action plans (Section V).

Table III. Key V&V Categories and Adoption Barriers

Category	Barriers
Data, Parameters, Inputs	Limited availability of detailed, high-fidelity datasets • Relevant datasets are currently relatively sparse, making it difficult to perform accurate and robust validation
	Complexity of higher dimensionality of 1) multiscale materials structures and models, 2) materials behavior mechanisms and models
	Often missing fundamental understanding of underlying physics, i.e., physical conditions • Results in difficulty with calibrating parameters to compensate for missing data/mechanisms
Integrated Design of Models and Experiments	Co-designing experiments and models is rare in the MOM community. • Researchers are often unsure how to achieve reciprocity between models and experiments; i.e., applying models (apples) versus accurate and robust validation with experiments (oranges)
Resources & Incentives	Lack of motivation for providing details of V&V methods in many scientific publications (although a few publications do this) • No incentive to provide desired novel V&V insights
Workforce Development/ Education	Lack of educational content and communication to build understanding of V&V and Uncertainty Quantification (UQ) in the MOM community/ workforce

Recommendations and Action Plans

Seven high-priority, high level recommendations are provided and discussed in this report (Section IV), followed by five detailed action plans that were developed along with some key activities/ tasks that were suggested for each action plan (Section V). The high-priority recommendations are summarized in Table IV, which is reproduced below.

Table IV. High-Priority Recommendations
Create a 'best practices' document for V&V in the MOM community
Develop a series of benchmark problems
Incentivize presentation of V&V activities in scientific publications
Create programs to achieve future V&V compliance requirements
Develop uncertainty quantification (UQ) methods for hierarchical structures and models
Demonstrate the value of V&V for industrial problems/products
Create V&V curricula/courses

The action plans and detailed tasks within each action plan are summarized in the list below, which is reproduced from section V of this report.

Action Plan 1:

Combinatorial Algorithms and UQ Methods for Multiscale Structures and Models

1.1. Conduct a robust study on development of key combinatorial V&V techniques for UQ
1.2. Develop high-fidelity multiscale methods for handling high-dimensional-parameter spaces
1.3. Fund a collaborative effort for a state-of-the-art review paper

Action Plan 2:

State-of-the-Art V&V: Analysis & Best Practices Document

2.1. Convene a working group of modelers, experimentalists, UQ experts, etc.
2.2. Identify best practices (i.e., V&V steps) in/for MOM community
2.3. Publish document/article of state-of-the-art V&V methods

Action Plan 3:

Series of Benchmark Examples & Challenge Competition

3.1. Form interdisciplinary benchmark teams and identify key benchmark challenges
3.2. Define scope and specifics of the benchmark problems
3.3. Launch benchmark challenge competition
3.4. Select data repository facility to house benchmarking information

Action Plan 4:

Multidisciplinary Training & Curricula Development

4.1. Fund development of V&V training programs for the MOM community
4.2. Launch tutorials/ workshops/ short courses
4.3. Modify existing university courses to include V&V topics
4.4. Develop new courses
4.5. Share and/or help create example benchmark problems

Action Plan 5:

Other V&V Framework Elements for Community Outreach, Adoption, and/or Compliance

5.1. Encourage/provide funding for large-scale collaborative grants
5.2. Promote a new breed of multiscale experiments for validation
5.3. Organize joint sessions/conferences on V&V
5.4. Catalogue and coordinate key experts for MOM V&V

For each of the tasks further consideration and discussion was provided including timeframes, personnel or affiliation types needed for that activity, metrics of success, rough cost estimates, and potential sources of support.

Final Call to Action

There is a great opportunity for the widespread adoption and implementation of critically needed V&V activities to enable accurate and quantitative predictive computational modeling associated with the MOM, which can in turn help accelerate new materials and manufacturing innovations. However, there is still much work to be done. As stated in the final section of this report, scientists, engineers, designers, policy makers and others who read this report are implored to use the information provided here to take direct action in order to help jumpstart and accelerate the widespread adoption and implementation of such V&V activities. Readers could begin to act upon many of the recommended action plans and activities in this report almost immediately by performing or contributing to specific research and/or development efforts; providing fiscal support for some of the recommended activities; or getting involved in some of the conference, publication, and/or educational activities suggested here.

I. Introduction

Predictive computational models associated with the MOM can help enable strong reductions in the cost and time for the development of new materials and products.[2,3] Over the past two decades, national initiatives have leveraged significant federal investment to accelerate the design of advanced materials through integrated computational/experimental approaches.[3,4] With the success of these initiatives, the use of computational models, tools, and techniques has become ubiquitous within the materials and mechanics communities. In this regard, as the value of predictive computational models for reducing time and cost of developing new mechanical structures, materials systems, and manufacturing technologies continues to grow, the widespread need for verification and validation (V&V) of these models cannot be overestimated. For example, Cowles et al. discussed the critical need for systematic procedures and widespread implementation of V&V as related to Integrated Computational Materials Engineering (ICME).[5] They pointed out that despite some progress in the development of V&V guidelines in fields such as fluid dynamics[6] and computational mechanics,[7] there is still a great need for widespread adoption and implementation of thorough and accurate V&V in other fields. Recent TMS studies[8,9,10] have also underscored the strong need for V&V in computational modeling in the mechanics and materials science and engineering communities.

Some very brief definitions of verification and validation offer a useful initial context:[1,6]

- **Verification** is the process of determining that a computational model accurately represents the underlying mathematical model and its solution.
- **Validation** is the process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model.

More detailed and broad ranging definitions of verification, validation, and uncertainty quantification (which is a key component of V&V) have been provided in a National Research Council (of the National Academies) report on *Assessing the Reliability of Complex Models: Mathematical and Statistical Foundations of Verification, Validation, and Uncertainty Quantification*:[11]

- *Verification.* The process of determining how accurately a computer program ("code") correctly solves the equations of the mathematical model. This includes code verification (determining whether the code correctly implements the intended algorithms) and solution verification (determining the accuracy with which the algorithms solve the mathematical model's equations for specified Quantities of Interest (QOIs)).
- *Validation.* The process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model (taken from AIAA, 1998[6]).
- *Uncertainty quantification (UQ).* The process of quantifying uncertainties associated with model calculations of true, physical QOIs, with the goals of accounting for all sources of uncertainty and quantifying the contributions of specific sources to the overall uncertainty.

The workshop participants conducted a thorough examination of existing definitions of V&V provided by a number of key organizations, and considered further ones that might be especially relevant for scientists and engineers working in the mechanics of materials (MOM) domain—see Section 2 below.

While the functionality and utility of predictive computational models associated with the MOM has grown dramatically within the last couple of decades, accurate and robust experimental validation of these models has generally lagged far behind. More specifically, although several efforts have expanded upon the need for V&V in science and engineering related to the MOM,[4–10] robust V&V has not been implemented as an integral and rigorous part of the scientific process supporting predictive computation and simulation in this domain as it has not been an area of strong or widespread focus in the relevant communities.

There is a foundation in other communities on which to build, such as the detailed V&V research and implementation work of researchers in electrical engineering and computer science;[12] fluid mechanics/dynamics,[13,14] validation, uncertainty estimation and/or optimization departments,[13,14] and other technical domains including computational engineering, physics, and/or the medical field. These researchers have covered topics such as: paradigms that relate V&V to the model development process, and recommended procedures for model validation;[12] practical frameworks, research needs, and management issues in V&V;[13] a review of V&V in computational fluid dynamics (CFD);[14] methods and procedures for assessing V&V, and some fundamental issues in V&V such as code verification versus solution verification, model validation versus solution validation, and the distinction between error and uncertainty.[14]

This workshop and report were organized to help chart a course for widespread adoption of robust V&V amongst both computational modelers and experimentalists in MOM, materials science, and other engineering disciplines by taking advantage of the foundation that has already been laid in

V&V in a variety of communities.[5–7, 11–15] To this end, the project approach consisted of recruiting and convening 40 subject matter experts (see Acknowledgments section) covering the wide range of expertise mentioned previously, for a one day, interactive, professionally facilitated workshop held July 27, 2018 in New York, NY, adjacent to the 13th World Congress on Computational Mechanics. Table I provides a summary of the workshop activities.

Table I: Summary of Workshop Activities
Scope and Definitions for Verification & Validation (V&V)
Identify and Prioritize Adoption Barriers of V&V Approaches in the Mechanics of Materials Focus Question: What barriers are preventing the adoption of comprehensive/rigorous V&V approaches within the mechanics of materials (MOM) community?
Identify and Prioritize Recommendations to Enable V&V Adoption Focus Question: Given these adoption barriers, what are the biggest opportunities to enable the rapid adoption and progress of V&V within the MOM community?
Identify Actionable Tactics to Implement Recommendations Focus Question: What 3-4 specific tactics are realistically needed to implement the key recommendations identified?

Most of the content of this final report was developed during these interactive, professionally facilitated sessions. These sessions consisted of some exercises involving the entire workshop group, and others involving breakout groups. The final workshop findings are provided in the following sections of this report:

- Barriers to V&V Adoption
- Opportunities and Recommendations
- Tactical Action Plans

Following the assembly of a draft report, a separate review team provided comments and suggested edits on that draft. This team consisted of some workshop participants as well as experts who did not attend the workshop.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II. Study Scope and Definitions of V&V

In 2012, the National Research Council published a report titled *Assessing the Reliability of Complex Models: Mathematical and Statistical Foundations of Verification, Validation, and Uncertainty Quantification*, which considered the mathematical sciences foundations of verification, validation, and uncertainty quantification (VVUQ), and recommended steps that will lead to improvements in VVUQ capabilities.[11] The study charge included the examination of practices for VVUQ of large-scale computational simulations across several research communities; identification of common concepts, terms, approaches, tools, and best practices; identification of mathematical sciences research needed to establish a foundation for continued development of the science of verification and validation (V&V) and uncertainty quantification (UQ) and for improving the practice of VVUQ; and recommendations for educational changes needed in the mathematical sciences community, and in mathematical sciences education needed by other scientific communities, to most effectively use VVUQ. That report[11] is highly recommended as a tour-de-force on the mathematical sciences foundations of V&V and UQ, and is not limited to a specific research community or domain.

As stated in the introduction, the workshop and report presented here have been focused on contributing to the widespread adoption/implementation of robust V&V in communities working with computational models specifically associated with the MOM (particularly solid materials), an area in which V&V is relatively immature. This is especially true when compared to other domains, such as aeronautical and nuclear industries, from which the V&V foundation already laid can be widely leveraged.

To provide a technical and contextual foundation for V&V in the MOM, the workshop participants first discussed the established definitions of V&V from a number of organizations. Several science and engineering professional societies have provided slightly different definitions for V&V, as shown in Table II. It was suggested that the American Society of Mechanical Engineers (ASME),[1] which builds upon the American Institute of Aeronautics and Astronautics (AIAA) definition,[1] provides one of the most useful definitions in the present context (see Table II), i.e., with respect to encouraging V&V adoption within the mechanics of materials (MOM) community.

Table II: Definitions of V&V from some key organizations

Source	Verification	Validation
ASME[1]	The process of determining that a computational model accurately represents the underlying mathematical model and its solution. • **Verification** is the domain of mathematics and validation is the domain of physics. • **Code Verification**—establish confidence, through the collection of evidence, that the mathematical model and solution algorithms are working correctly. • **Calculation Verification**—establish confidence, through the collection of evidence, that the discrete solution of the mathematical model is accurate.	*(identical to below AIAA definition⇃)*
AIAA[6]	The process of determining that a model implementation accurately represents the developer's conceptual description of the model and the solution to the model	The process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model
IEEE[16,17]	The process of evaluating the products of a software development phase to provide assurance that they meet the requirements defined for them by the previous phase.	The process of testing a computer program and evaluating the results to ensure compliance with specific requirements
MITRE[18]	Verification can be defined as finding and eliminating errors in numerical algorithms/codes and evaluating the solution accuracy of numerical methods against design requirements by comparing with highly accurate or closed-form benchmark solutions.	Validation is the process of determining the degree to which a model accurately represents reality (the experiments) within the range of intended use.

NASA[19]	Verification is the process for determining whether or not a product fulfills the requirements or specifications established for it.	Validation is the assessment of a planned or delivered system to meet the sponsor's operational need in the most realistic environment achievable.
National Research Council[11]	The process of determining how accurately a computer program ("code") correctly solves the equations of the mathematical model. This includes code verification (determining whether the code correctly implements the intended algorithms) and solution verification (determining the accuracy with which the algorithms solve the mathematical model's equations for specified Quantities of Interest (QOIs))	*(identical to above AIAA definition↓)*

To provide the readers of this report with further context as to both the definitions and the utility of verification and validation, the workshop participants also developed a list of questions and comments for both modelers and experimentalists to consider when they contribute to and/or use computational models associated with the MOM. Some key questions they suggested that may help capture the essence of model verification include: (1) Are you solving equations the correct way? (2) Are you implementing the requirements correctly? (3) Does the model behave the way you expected? Some key questions and statements that relate to validation are: (1) Are you solving the right equations? (2) How are you doing the comparison to experiments? (3) To validate your model, does it need to connect to the reality of interest? A related question could be: Is the model representative of reality and how do you define that reality? (4) Uncertainty quantification cannot be separated from validation approaches; one must quantify the uncertainty of the prediction. (5) It is crucially important to define validation metrics. In this regard, even disciplines in which V&V is more mature, such as computational fluid dynamics (CFD), often do not have a good command of such metrics and statistical methods may be needed.

Finally, given the aforementioned suggestion that the ASME definition of V&V best serves the purposes of the present study, a well-known flow chart published by ASME provides a visual depiction of the V&V process that includes uncertainty quantification for modeling and experimental activities (see Figure 1).[7]

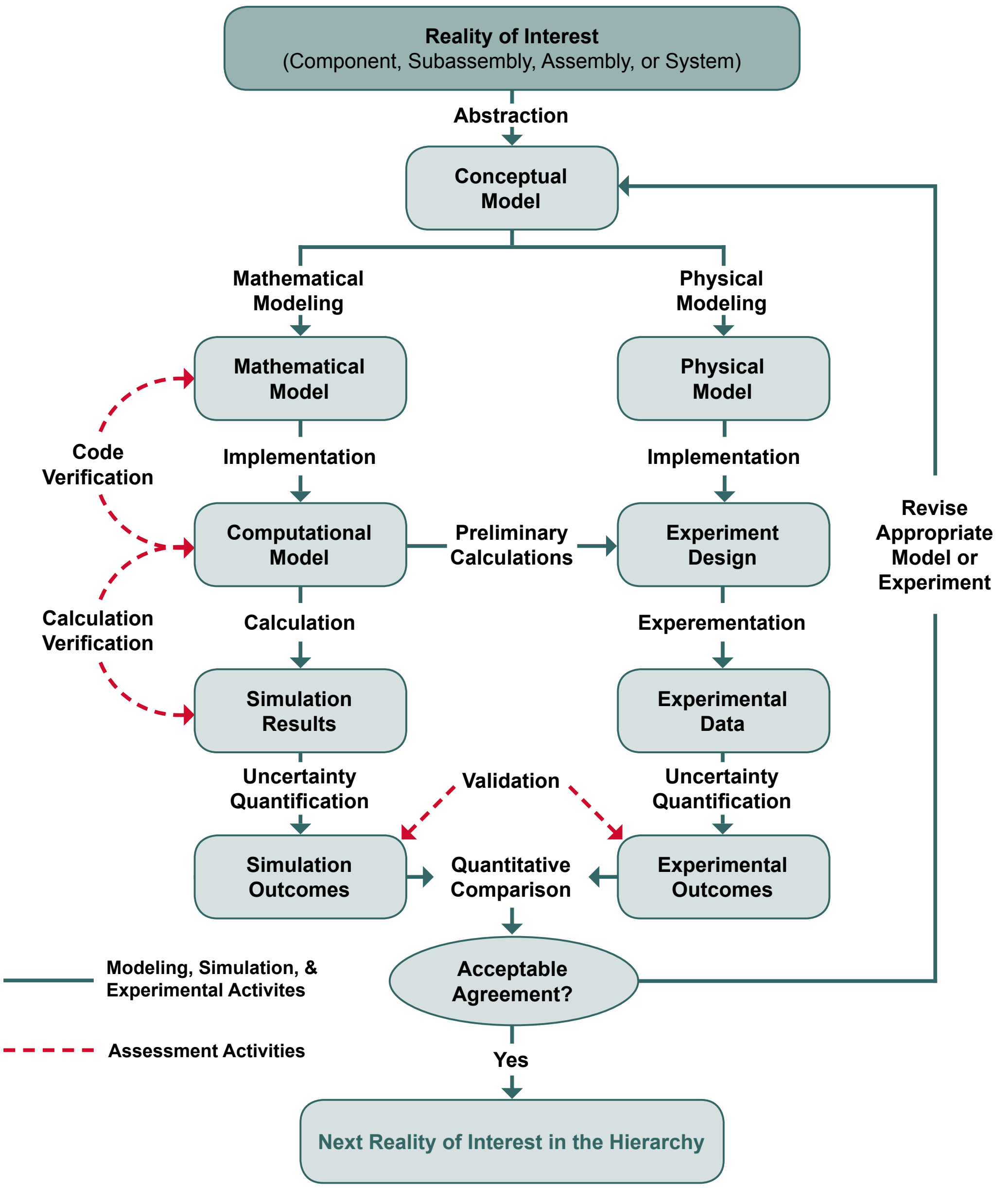


Figure 1: Flowchart depicting the various activities and outcomes of the V&V process (Reprinted from ASME V&V 10-2006 (R2016), by permission of The American Society of Mechanical Engineers. All rights reserved.)[7]

Having considered the definition and scope of V&V in the MOM domain, the barriers that have prohibited the widespread adoption of V&V in the associated communities are considered in Section 3, followed by recommendations and detailed action plans in Sections IV and V, respectively.

III.
Barriers to V&V Adoption

Building upon the various verification and validation efforts underway in other science-related fields, the workshop participants were charged with identifying what they viewed to be the most significant barriers preventing the adoption of rigorous V&V approaches within the mechanics of materials (MOM) community. These barriers were identified both to assist the MOM community in the comprehensive adoption and implementation of robust V&V methodologies, and to provide a foundation from which the team could develop broad recommendations and detailed action plans for overcoming these barriers (Sections IV and V).

Due to the diversity of computational methods used throughout the mechanics and materials communities, stimulating widespread and robust V&V requires addressing numerous technical, cultural and policy-related challenges. The workshop participants compiled a prioritized list of some key overarching challenge categories, shown in the first column of Table III. These represent the largest impediments to widespread adoption. The table also provides the most significant barriers that need to be addressed within each of the broad challenge categories. Beyond the prioritized barriers presented in Table III, a full table of all identified categories (8) and barriers (31) is presented in Appendix A.

Table III. Key V&V Categories and Adoption Barriers	
Category	Barriers
Data, Parameters, Inputs	Limited availability of detailed, high-fidelity datasets • Relevant datasets are currently relatively sparse, making it difficult to perform accurate and robust validation
	Complexity of higher dimensionality of 1) multiscale materials structures and models, 2) materials behavior mechanisms and models
	Often missing fundamental understanding of underlying physics, i.e., physical conditions • Results in difficulty with calibrating parameters to compensate for missing data/mechanisms
Integrated Design of Models and Experiments	Co-designing experiments and models is rare in the MOM community. • Researchers are often unsure how to achieve reciprocity between models and experiments; i.e., applying models (apples) versus accurate and robust validation with experiments (oranges)
Resources & Incentives	Lack of motivation for providing details of V&V methods in many scientific publications (although a few publications do this) • No incentive to provide desired novel V&V insights
Workforce Development/ Education	Lack of educational content and communication to build understanding of V&V and Uncertainty Quantification (UQ) in the MOM community/ workforce

The categories and barriers in Table III are considered further below, particularly as they relate to the mechanics and materials communities.

Data, Parameters, and Inputs

Issues related to the limited availability of data (including relevant metadata) and poor integration of data analytics approaches for the generation of surrogate models are seen as some of the largest barriers to V&V adoption in the MOM community. High-fidelity, physics-based models used during product development and manufacturing are often of high complexity and demand physically accurate inputs and parameters to produce meaningful results. Moreover, the complexity related to the higher dimensionality of materials structures and/or models that span many materials, length/time scales, and materials behavior mechanisms that include an extremely large number of variables, all lead to exponentially more parameters and model forms. The difficulty in identifying and/or obtaining appropriate parameters and inputs often results in models that do not fully account for the system behavior, leading to more difficult verification and validation, particularly in models that are significantly complex. The lack of widely available, detailed, high-fidelity experimental datasets further exacerbates this barrier as it severely limits the community's ability to perform rigorous calibration and validation.

Integrated Design of Models and Experiments

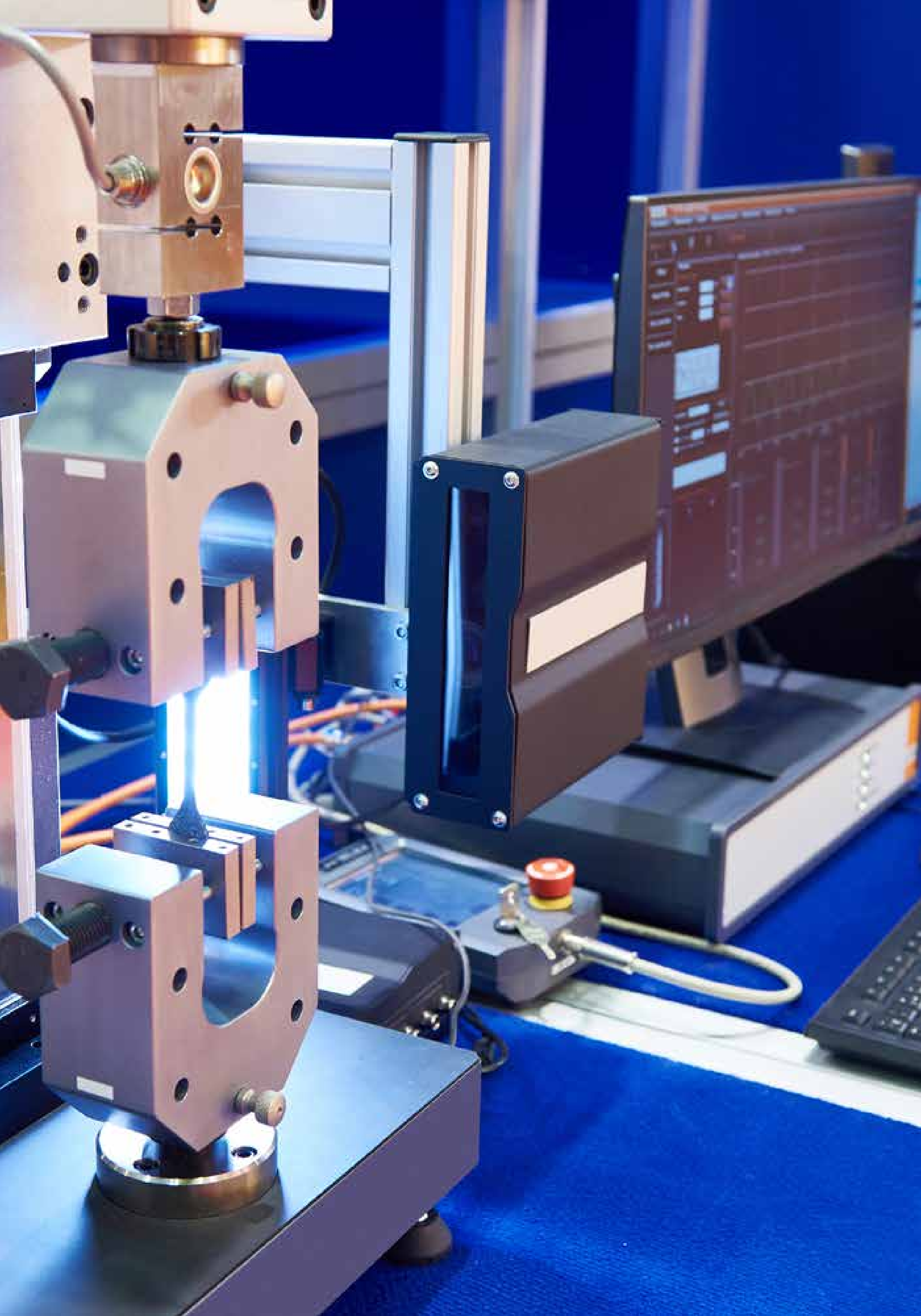
Traditionally, targeted experiments are used to obtain realistic input and/or time-dependent values for improved accuracy of and comparison to models and simulations. However, due to complexities in the models employed throughout the materials and mechanics communities, it is challenging 1) to measure all of the appropriate model parameters and 2) to integrate all necessary targeted experiments for sub-models. Moreover, the output from models often predicts mechanical behaviors that are difficult to fully capture experimentally, thus limiting means of validation. More purposeful co-designing of experiments and models earlier in the project lifecycle would represent a significant step toward enabling V&V throughout the MOM community.

Resources and Incentives

Another major impediment is the absence of V&V related incentives and resources within the MOM community. As previously mentioned, the sparse availability of relevant datasets often makes it difficult and expensive to perform meaningful validations and compare different models. In addition, the lack of shared and accessible data repositories containing both experimental and modeling data leads to variations and deficiencies in the types of data and metadata collected, which in return restricts the V&V methods available to the individual researcher. The issues surrounding the dearth of resources are magnified by the lack of incentives to provide V&V related outputs. Most scientific publications currently have little to no requirements or incentives for providing details of V&V/UQ methods, and industrial companies are often discouraged from disclosing too many details due to proprietary practices. Although the current absence of clear, widespread publication incentives suggest the community is unlikely to organically develop the culture or resources necessary for a successful V&V foundation, a few journals are adopting V&V/UQ requirements, providing some optimism for progress, especially as other journals follow suit. On the other hand, the lack of V&V resources, tools, and data discourages V&V activity as it is often quite costly and time-consuming to employ rigorous V&V methodologies. In this vein, budgets for researchers and engineers in academia, government, and industry are already so tight that it is often difficult to justify the need for further resources beyond those required to sustain the existing project person-hour and capital costs. The lack of an adequate V&V data infrastructure and deficiency in proper communication of the great benefits of V&V in mitigating risk and accelerating technological innovation further magnify this impediment. In this regard, better education and communication of the benefits of V&V, and correspondingly the risks associated with not performing adequate V&V of predictive models, are needed to incentivize successful adoption.

Workforce Development/ Education

To achieve a strong V&V culture and adoption within the community, the MOM workforce at large will need to acquire new knowledge and skills. Currently, the materials and mechanics workforce is generally not well trained in areas such as statistics, uncertainty quantification, and data analytics and management, nor are these skills emphasized in current curricula. Cross-disciplinary educational opportunities that highlight these skills, be it through curricula reform or post-graduate training, are needed to help build the necessary understanding of V&V and throughout the MOM community and workforce, yet such opportunities are presently very rarely available.



IV. Opportunities and Recommendations

Once the most significant barriers and needs preventing the adoption of rigorous V&V approaches within the MOM community were identified, the workshop participants were tasked with identifying the greatest opportunities available to enable rapid adoption and progress of such V&V approaches and then prioritize the most significant opportunities and solutions, i.e., provide key recommendations for stimulating rapid progress within the MOM community.

The following overarching opportunity areas were first identified:

- Benchmarking and best practices
- Multidisciplinary programs and initiatives
- Data repositories and toolsets
- Incentivization of V&V
- Sensitivity analysis and uncertainty quantification
- Making a strong value proposition for V&V
- Workforce development

Based on these opportunity areas, some broad recommendations were developed, from which those deemed of the highest priority and/or most promise were selected in order to subsequently develop highly detailed action plans (see Section V). The full list of recommendations is presented in Appendix B, while those of highest priority are summarized in Table IV and discussed below.

Table IV. High-Priority Recommendations
Create a 'best practices' document for V&V in the MOM community
Develop a series of benchmark problems
Incentivize presentation of V&V activities in scientific publications
Create programs to achieve future V&V compliance requirements
Develop uncertainty quantification (UQ) methods for hierarchical structures and models
Demonstrate the value of V&V for industrial problems/products
Create V&V curricula/courses

It should be noted that various other recommendations, provided in Appendix B, had areas of overlap with the high-priority recommendations, and some of these overlap areas are melded into the discussion below.

Create a Best-Practices Document for V&V in the MOM Community

A critical first step in stimulating widespread implementation of V&V in the MOM community is to develop a state-of-the-art V&V best-practices document specifically for researchers, engineers, and designers who perform work associated with computational modeling of MOM. Such a document should include a tutorial of how to frame V&V practices, as well as provide the minimum standard for UQ/sensitivity analyses, as applied specifically to models and/or problems within the MOM domain. In other words, this document should also address the following question for scientists and engineers: What is the ‘minimal’ set of requirements for rigorous V&V of problems or models being undertaken in this community? Best practices from other disciplines and sub-disciplines should be leveraged, but the practices developed and documented here should focus more specifically on predictive computational models directly associated with the MOM systems and structures. The goal is for this document to be a “field manual” of sorts for modelers, experimentalists, and other domain specialists working in this area, including both those that have some experience with V&V and those that have little or no experience. At the very least, it should help raise awareness of V&V practices in the solid mechanics, and materials science and engineering communities.

Develop a Series of Benchmark Problems

Benchmark problems can expose and/or clarify good V&V practices in a specific technical domain. Therefore, it is important to launch a series of benchmarking studies geared toward MOM computational modeling. Each benchmark study should have very clearly defined materials, material properties, tests, and test specimen geometries, as well as detailed descriptions of the required statistics of test data, e.g., in the form of mean values with error bars and/or a distribution. It is critical that these benchmarking problems are undertaken on focused and interpretable ‘unit tests’, rather than designed for a problem of high complexity, so that modelers across different research groups can directly and objectively compare final results and assess the V&V approaches employed. In this way, these benchmark problems may pave the pathway toward more optimized and efficient

V&V practices as well as create a platform for the community to learn from each other. As more benchmark problems and challenges are executed and documented, the outputs can be incorporated in any V&V best practices documents, which could be continually updated and improved upon.

One past effort that reached into the MOM community is the series of Sandia Fracture Challenges,[20,21,22] in which researchers and engineers were invited to predict crack initiation and propagation in a simple geometry fabricated from a common alloy. The specific goal of this international challenge has been to benchmark capabilities for the prediction of deformation and damage evolution associated with ductile tearing in structural metals. The resultant wide variation in modeling outcomes showed a striking range of predictions across research groups and indicates a strong need for robust and accurate V&V for computational modeling of the ductile fracture of metals.[20,21,23] Another recent (2017) example was focused on modeling of the additive manufacturing process from feedstock to finished parts. TMS and the National Institute of Standards and Technology (NIST) partnered to run Additive Manufacturing Benchmarks 2018 (AM-Bench 2018). This was the first in a planned series of events focused on validating and improving the accuracy of model predictions and developing universally accepted quantitative measurement approaches for additive manufacturing (AM) materials and methods.[24] Similar benchmarking efforts within the MOM domain could strongly support implementation of more accurate and robust V&V within the community. Ultimately, a V&V database of benchmark problems and results might be developed, specifically for access by the MOM community.

Incentivize Presentation of V&V Activities in Scientific Publications

As alluded to in section 3, there is a dearth of resources in support of widespread V&V in the solid mechanics and materials science and engineering communities, and this deficiency is magnified by the lack of incentives to perform robust V&V. In this vein, science and engineering journals offer a great opportunity to provide incentives since publication is strongly encouraged in academia and national laboratories, and, perhaps to a lesser extent, in industry (for proprietary reasons). Although some journals, such as *Data in Brief, SoftwareX, Journal of Open Source Software,* and *Integrating Materials and Manufacturing Innovations* incentivize code and/or data sharing, and thus may stimulate more V&V activity, very few journals strongly encourage and/or require consideration of V&V content. It is recommended that editorial boards and publishers of journals that attract relevant articles involving computational modeling start to develop such requirements, especially V&V activities that ensure higher quality modeling efforts and publications. This could in turn result in higher citations, impact factors, and greater readership, all of which are valued by these journals. Owing to the aforementioned incentives for scientists and engineers to publish, this would incentivize stronger and more widespread V&V activities.

Create Programs to Achieve Future V&V Compliance Requirements

Journals could provide some type of framework or guidance to help modelers and experimentalists achieve V&V compliance requirements. For instance, they could provide publication standards for metadata, experimental results, and/or simulation results (e.g., checklists, technical requirements, stating of key assumptions), with a focus toward making the scientific results more reproducible, especially via proper V&V. Since most project budgets and time availability of researchers and engineers are already spread very thin coupled with the fact that it is costly and time-consuming to employ rigorous V&V methodologies, publication efforts need to be leveraged with other incentives as well. These could include V&V requirements for funding supporting predictive modeling. For instance, agencies and funding officers could set V&V requirements in germane funding opportunity announcements and/or open call proposals involving computational modeling, such that researchers (both modelers and experimentalists) would have to show at least some plan for addressing V&V. This could provide very strong incentive for learning about and more strongly addressing V&V. As an example in a different but related area, many agencies already require a plan for managing and storing the data that is generated from research programs.

Develop Uncertainty Quantification Methods for Hierarchical Structures and Models

Uncertainty quantification (UQ) techniques are a linchpin for V&V, and uncertainty can particularly dominate the reliability (or unreliability) of results for multiscale models. In this regard, uncertainty can grow as data (both experimental and computationally modelled) is propagated across length and/or time scales. One tactic is to develop combinatorial techniques for determining and quantifying uncertainty across length scales. Error bounds should be required on both measured and modeled datasets at all length and time scales. Properly tackling UQ and sensitivity analyses for hierarchical models will also require multidisciplinary programs and initiatives. One example is long-term multi-agency initiatives for dedicated V&V research and/or education across solid mechanics, materials, statistics, mathematics and/or computer science disciplines. Such initiatives could support interdisciplinary research groups involving multiple principal investigators and could make vast in-roads toward widespread adoption of V&V.

Demonstrate the Value of V&V for Industrial Problems/Products

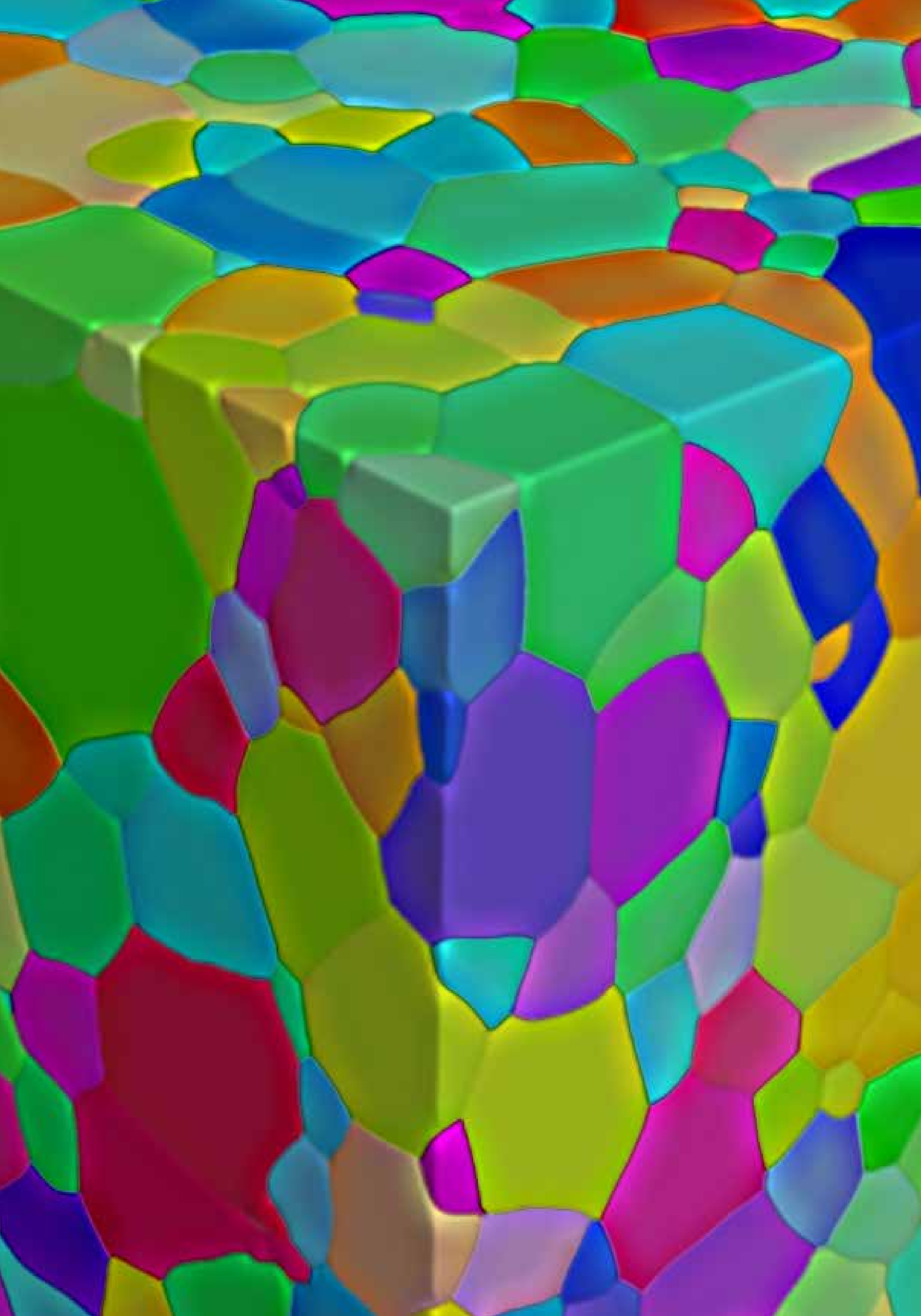
Making a strong value proposition is foundational for incentivizing robust and widespread V&V in the solid mechanics and materials science and engineering communities. Demonstrating the value of V&V on "real-life problems," which are relatable to a wide range of stakeholders across the broader society, can be especially impactful. For instance, it needs to be widely communicated that accurate V&V of predictive MOM models has great value as related to the ability of these models to reduce the time and cost of developing new consumer products and manufacturing methods, as well as to improve the product quality, lifetime, and cost for both new and existing product lines. It is equally important to communicate the negative consequences and risks of not doing proper

V&V of predictive models, including the potential for contributing to disastrous product failures (for instance in the aerospace or automotive industries). Specific case studies and examples will be of great value here.

By utilizing various communication platforms, including publications, conferences, symposia, classrooms, professional society committees, and social media, V&V champions should communicate this value proposition much more widely in the solid mechanics, materials science and engineering, and related science and/or engineering communities. This will in turn help transition the perception of V&V away from being viewed as an area of interest to a recognition that it is a sub-discipline that must permeate all computational modeling, including in the area of the MOM.

Create V&V Curricula/Courses

For thorough V&V to take off more broadly and sustainably among those working with computational models associated with MOM, education of the current and future workforce, and future teachers, is essential. Development of V&V educational curricula at universities as well as continuing education courses offered by professional societies, industry, or other organizations could eventually make V&V a commonplace technique for both modelers and experimentalists in the materials science and engineering and solid mechanics communities. Likewise, tutorials and educational plenary talks at major conferences that attract MOM modelers and experimentalists could be of great value in providing some of the basic underpinnings and utility of V&V, which could entice people to learn more. Potential conferences for such tutorials/presentations include those associated with the mechanics community, materials scientists and engineers, mechanical engineers, the manufacturing community, mathematicians, statisticians, and/or computer scientists.



V.
Action Plans

Based on the opportunities and recommendations discussed in Section IV, five high-priority action plans were developed and some key activities/tasks were suggested for each action plan. For each task, consideration was given to issues such as timeframe, personnel or affiliation types needed to lead or participate, metrics of success and/or milestones, rough estimates of cost, and potential sources of support. The Action Plans and Key Tasks are summarized below (in no specific order of priority):

Action Plan 1:
Combinatorial Algorithms and UQ Methods for Multiscale Structures and Models

1.1. Conduct a robust study on development of key combinatorial V&V techniques for UQ
1.2. Develop high-fidelity multiscale methods for handling high-dimensional-parameter spaces
1.3. Fund a collaborative effort for a state-of-the-art review paper

Action Plan 2:
State-of-the-Art V&V: Analysis & Best Practices Document

2.1. Convene a working group of modelers, experimentalists, UQ experts, etc.
2.2. Identify best practices (i.e., V&V steps) in/for MOM community
2.3. Publish document/article of state-of-the-art V&V methods

Action Plan 3:
Series of Benchmark Examples & Challenge Competition

3.1. Form interdisciplinary benchmark teams and identify key benchmark challenges
3.2. Define scope and specifics of the benchmark problems
3.3. Launch benchmark challenge competition
3.4. Select data repository facility to house benchmarking information

Action Plan 4:
Multidisciplinary Training & Curricula Development

4.1. Fund development of V&V training programs for the MOM community
4.2. Launch tutorials/ workshops/ short courses
4.3. Modify existing university courses to include V&V topics
4.4. Develop new courses
4.5. Share and/or help create example benchmark problems

Action Plan 5:
Other V&V Framework Elements for Community Outreach, Adoption, and/or Compliance

5.1. Encourage/provide funding for large-scale collaborative grants
5.2. Promote a new breed of multiscale experiments for validation
5.3. Organize joint sessions/conferences on V&V
5.4. Catalogue and coordinate key experts for MOM V&V

Action Plan 1: Combinatorial Algorithms and UQ Methods for Multiscale Structures and Models

Task 1.1

A key task needed in developing combinatorial algorithms and UQ methods for multiscale MOM models is to conduct a robust research effort involving both modeling and experiments. Within the first six months to a year of this task an important first step is to identify key sources of uncertainty for such models. In the longer term (~3–5 years), novel stochastic techniques to handle large, sparse datasets associated with hierarchical MOM models need to be developed and fully demonstrated. In parallel, experimental characterization and testing at different length scales should be conducted to support these efforts; error bounds should be required on both measured and modeled datasets. Uncertainty qualification methods employed should be verified using convergence, error estimation, etc. Some metrics or milestones to measure progress of this task include publications that result throughout this effort, and at the latter stages development of a robust database of both experimental and computational results that could serve as a V&V resource to the solid mechanics, materials science and engineering, and related communities. This task would likely be conducted by researchers in academia and/or national laboratories, and funding support could be provided by government agencies. It is very roughly estimated that the level of support needed for such an effort would be on the order of $3M–$5M.

Within the first six months to a year of this task an important first step is to identify key sources of uncertainty for such models. In the longer term (~3–5 years), novel stochastic techniques to handle large, sparse datasets associated with hierarchical MOM models need to be developed and fully demonstrated.

Task 1.2
This activity is related to Task 1.1, but would especially target multiscale UQ methods, i.e., across nano-micro-meso-macro length scales. It would involve development of optimization algorithms suitable for high-dimensional parameter spaces and should leverage artificial intelligence (AI) approaches such as machine learning (ML), applied within the physics constraints associated with solid mechanics and materials models. Leveraging Task 1.1, statistical data assimilation of multiscale/multiphysics experimental measurements should be undertaken to enhance uncertainty prediction and provide validation databases for the UQ methods developed. Finally, key high-performance computing (HPC) resources should be identified and utilized to support the large data volumes associated with multiscale methods and high-dimensional-parameter spaces, as required for effective UQ in this task. Completion of this effort could take 3–6 years; some metrics to measure progress include the ability of the algorithms to handle high dimensional parameter spaces as well as the successful deployment of these capabilities across a variety of application spaces. This type of work is best accomplished within academia, across a variety of disciplines and/or sub-disciplines including computer science, statistics, and mathematics, with guidance by researchers in solid mechanics, materials science and engineering, and related fields. Support on the order of $3M–$5M is estimated for this effort as well.

Task 1.3
A relatively short-term task supporting this action plan that could be attacked early on would be to fund a collaborative effort to undertake a state-of-the-art review paper or set of such papers in this arena. This review could be used as a resource for the other tasks, and would involve collaboration between experts contributing to this area from various key disciplines, including computer science, computer engineering, statistics, solid mechanics, and/or materials science and engineering. It could be supported by a relatively low level of "glue funding" (perhaps $100K–$300K) supplied by a government agency(ies).

Action Plan 2: State-of-the-Art V&V: Analysis & Best-Practices Document

Task 2.1
The first task would be for one or more organizations (perhaps professional societies or publishers) to identify and convene an expert working group of modelers, experimentalists, V&V practitioners, UQ experts, and other specialists from various sub-disciplines, who have the background and experience to contribute to a highly impactful best-practices guidance document for V&V of MOM-related models. It should be a relatively diverse group of about 15 people or less, representing universities, government laboratories, and industry.

Task 2.2

The expert working group would identify V&V best practices for the MOM community. They could first determine current V&V practices associated with MOM models, then identify and reevaluate in more detail fundamental gaps, challenges, and opportunities for V&V adoption (starting with this report as a foundation). Strong case study examples of effective V&V in the community should also be identified. The group could then develop a document specifically for those working with models and/or problems associated with MOM. This document could review the value of and motivation for doing V&V, demonstrate different levels of V&V rigor (e.g., low, medium, high), provide some important case studies, highlight some applicable best practices from other disciplines and sub-disciplines, provide more targeted best practices, and cover any other areas that the expert working group members determine would best benefit members of the MOM community. The targeted readership within this community should include researchers and engineers who have some V&V experience, as well as those that have none.

Task 2.3

The organizations leading the study (e.g., the professional societies or publishers) would work with the subject-matter-expert team to write draft manuscript(s), then refine, produce, publish, and widely disseminate documents across the relevant communities, in order to provide the highest impact on stimulating more widespread and robust V&V activity across these communities.

Action Plan 3: Series of Benchmark Examples & Challenge Competitions

Task 3.1

The first task would be for one or more organizations to take the lead on organizing benchmark challenges and convening the interdisciplinary benchmark lead technical team(s). For the benchmark examples provided in Section 4,[20,21,24] these lead organizations included national laboratories and a professional society. Benchmark technical teams could then identify one or two benchmark problems for each challenge, all geared toward MOM computational modeling, with each benchmark study focused on three key groups: modelers, experimentalists, and V&V/UQ practitioners. It is important that the lead technical teams be composed not only of experts from the solid mechanics and materials science and engineering disciplines, but also computer scientists, UQ experts, and applied mathematicians. This will additionally help to convene potential future collaborations for other V&V activities.

Task 3.2

Once the lead organization, the technical team(s), and the key benchmark problems are in place, the scope and specifics of the benchmark problems can be developed for each challenge, typically by conducting the experiments (and/or preliminary modeling) that fully define specifics of the benchmark problems. If this has not been done previously in some research programs (by the technical team members or some other researchers), the team members for that challenge will need to conduct such tests/analyses in their own laboratories, which might take anywhere between six and twelve months to complete. The specifics might include the material(s), material properties, test type, test specimen geometries, and/or type of test result. It is important that the test conditions and parameters be very tightly constrained so that modelers in different research groups can directly compare their final results and VV/UQ methods, and to facilitate the elucidation of key modeling challenges for the MOM community.

Task 3.3

The first benchmark challenge competition will then be ready to launch. About one year in advance of the date of the conference or workshop where the final presentations are made and the modeling results are subsequently judged, the lead organization will have to disseminate targeted communications to the relevant communities, inviting entries to the competition as well as attendance and/or presentations at the final event. In addition to targeting these communications to the mechanics and materials science and engineering communities, the benchmark challenge could also be promoted via vehicles (websites and/or email lists) that are accessed specifically by computer scientists, mathematicians, and/or statisticians, with the added purpose of stimulating more interdisciplinary collaborations in this arena. The level of funding support required for such benchmark initiatives should be similar to that of any large workshop or small specialty conference. These costs are typically covered by some combination of attendee registration fees, federal agency support, and industrial sponsorship.

Task 3.4

When the benchmark challenge competition and final event are completed, it is very important that the rich modeling and experimental data generated is not lost, and in fact that it is made available to the community at large. This data is especially valuable since it was all generated for the same, very specific problem, and thus could be utilized for further V&V analyses and/or learning by many other researchers, beyond just those that participated in the benchmarking event. The benchmark metadata, experimental data, modeling inputs and outputs, and perhaps even the computation models should be housed in an existing repository, perhaps at one of the contributing or sponsoring organizations involved in this effort. The results of the challenge and location of the repository can then be published in a journal(s) with large readership by the MOM community, in order to provide for much greater impact toward adopting V&V across this community.

Action Plan 4: Multidisciplinary Training & Curricula Development

Task 4.1

Development of V&V training programs for the MOM community could be funded by government agencies (perhaps supplemented by industry). An existing government model, for example, that supports these types of training efforts and especially targets innovative, cutting-edge, interdisciplinary research areas, is the NSF Research Traineeship (NRT) Program.[25] Other government agencies may already have or could develop similar programs, and industrial companies might also contribute. Interdisciplinary teams of principal investigators could be formed to submit proposals for training associated with computational modeling of MOM, combined with capturing the requisite experimental information, with strong components focused on V&V. This would incentivize not only training for the direct implementation of V&V for MOM models, but the formation of collaborative interdisciplinary teams of researchers and educators needed to develop V&V methodologies for such models. Estimates of support levels required for the development of such training initiatives could vary greatly (i.e., $500K–$3M) depending on the length of the award (i.e., 2–5 years) and the size of the teams. Some metrics of success for the training programs developed are how well they are subsequently picked up and independently sustained by other organizations that offer such training (universities, professional societies, companies), and how many students ultimately attend such courses.

Interdisciplinary teams of principal investigators could be formed to submit proposals for training associated with computational modeling of MOM, combined with capturing the requisite experimental information, with strong components focused on V&V.

Task 4.2

A variety of tutorials, workshops, and/or short courses for working professionals and/or university students could be developed and executed by professional societies. Panels of experts could be convened to develop the technical content for and lead such courses/workshops, which would be held at mechanics-, materials science and engineering-, and/or V&V-related conferences. In some cases, multiple professional societies might coordinate (e.g., TMS, ASME, and/or AIAA) to hold the same course at their different meetings. The course materials developed from these efforts might also be the source of eventual book chapters or other educational initiatives (e.g., see the other tasks under Action Plan 4). There is already a well-developed model for such events by professional societies, in which the costs are covered by some combination of course registration fees, government agency support, and industrial sponsorship. These events could begin development after this report is published (March 2019), and thus could be executed as early as 12–18 months from then. Metrics of success could include number of attendees, fiscal soundness, recurrence/sustainability over time, course/workshop survey results, skill assessments conducted before and after events, number of different events executed, and impact of these initiatives on V&V adoption in the MOM community (as determined by surveys and/or studies continuing for years after the event).

Task 4.3

Within universities, one possibility is to modify existing university courses which are taught to students in mechanical engineering, materials science and engineering, and other departments related to MOM. These modifications would include adding content related to both computational and experimental methodologies used to support V&V. Undergraduate courses could focus more on educating students as to the value of V&V (or more importantly the pitfalls of not doing V&V), some of the tools and methodologies that are required and available, and how some of these techniques work. Graduate course content could focus on application/implementation of V&V and statistical analyses in specific technical focus areas. Content could begin to be developed as soon as some champions for these efforts within universities begin to step forward (perhaps after reading this report), and could be implemented within one to two years. As with other V&V initiatives, interdisciplinary collaborations and buy-in across university departments (e.g., mechanical engineering, materials science and engineering, statistics, computer science, mathematics, and/or electrical engineering) would be of great value. Metrics of success might include the number of courses modified, to what extent the courses were modified, student surveys, and pre- and post-assessments of students' skills.

Task 4.4
This task is similar to Task 4.3, but is centered about the development of new courses rather than modification of existing courses. Most of the considerations in Task 4.3 would apply here as well, but this task would take considerably more buy-in, approval, effort, and incentivization. An entire course in this domain would center on approaches and best practices for V&V of scientific/engineering models. Lectures, homework assignments, and exams could borrow from the best practices document from Action Plan 2 and the benchmark problems from Action Plan 3. Such a course could also involve teaching some statistics concepts and UQ and would likely be on the graduate level. Interdisciplinary/interdepartmental collaborations on such a course could be especially valuable and such interactions might spill over to the additional benefit of professors co-advising on student research projects and/or theses. Success metrics would include the number of new courses developed, their longevity, course attendance figures, student surveys, and pre- and post-assessments of students' skills.

Task 4.5
Related to and/or in conjunction with Action Plan 3, example benchmark problems could be created and shared, in this case with the specific purpose to serve as educational resources for students and/or professionals to learn V&V approaches. Case studies and examples could be used as teaching materials, and short mock/virtual/"mini" challenges could be executed via working teams within a classroom setting. These educational resources could be employed in both the university curricula and professional development courses and workshops described in tasks 4.1–4.4 above.

Action Plan 5: Other V&V Framework Elements for Community Outreach, Adoption, and/or Compliance

Task 5.1
A critical element contributing to a "framework" for widespread adoption of rigorous V&V for MOM models is funding for large-scale collaborative grants. In many of the other opportunities (Section IV) and action plans and tasks (Section 5) discussed elsewhere in this report, the need for interdisciplinary collaboration and incentivization has been emphasized. Although the value of implementing rigorous V&V (as well as the risks and pitfalls of ignoring V&V) has been discussed repeatedly throughout this report, funding must be made available to incentivize and allow scientists, engineers, and designers to develop and implement specific V&V and UQ methodologies because these can be very time consuming and costly. Large-scale grants are estimated here to be on the order of $10M or more to adequately support a number of collaborative researchers and their resources (computer hardware, software, experimental and testing equipment) for the requisite number of years to develop and implement these techniques, while also providing large volume data generation, management, storage, and sharing. Such efforts will likely require collaboration amongst multiple divisions and directorates within a given government agency, and in some cases possibly across different government agencies, to coordinate and combine resources for specific funding calls/proposals. Metrics of success for this task will include the number, size, and lifetime of such grants. But much more important will be the subsequent impact of the funded programs, as measured by the resultant publications, presentations, computational models and codes, graduate degrees, courses, foundational and reusable data sets, and estimated product development cost and time savings (via accurate predictive models). Other less quantifiable metrics are also extremely important, such as the number of researchers/engineers/designers made aware of the value of V&V, and/or who, as a result of the program outputs, actually begins to implement V&V in MOM models.

Task 5.2

Beyond the many types of recommendations, action plans, and tasks mentioned above, an important element toward generation of high-quality, high-volume experimental characterization and test data needed for rigorous validation of multiscale (i.e., across length and time scales) MOM computational models is the development of new, innovative experiments[9] (see also tactic 1.1 above). High throughput experiments that develop large amounts of high-quality data in reasonable times will be sorely needed for proper V&V of such models. This could involve the development of totally new techniques associated with real-time measurements, and wherever possible, those measurements should be made simultaneously across multiple length scales.

An important element toward generation of high-quality, high-volume experimental characterization and test data needed for rigorous validation of multiscale (i.e., across length and time scales) MOM computational models is the development of new, innovative experiments.

Task 5.3

Symposia at large conferences, small specialty conferences, and/or workshops are all excellent ways to promote V&V adoption. Owing to the inherent interdisciplinary nature of implementing and operationalizing V&V, there is a great opportunity for such symposia, conferences, or workshops to be planned and/or executed collaboratively by professionally societies serving different disciplines - such as TMS, ASME, AIAA, the Institute of Electrical and Electronics Engineers (IEEE), and/or the American Society for Civil Engineers (ASCE). For example, joint sessions/programs could be organized by establishing volunteer organizing teams with member representation from each of the collaborating societies. Symposia could rotate between the large, annual conferences organized by these organizations, or smaller workshops or specialty conferences could be jointly planned and executed by multiple societies. In either of these scenarios, cross marketing and communications could be coordinated for these events. There are well-established models for such coordination among societies serving similar communities;[26,27] this is not as common across more differentiated science and/or engineering disciplines. Costs for such events would typically be covered by some combination of attendee registration fees, federal agency support, and/or industrial sponsorships. Planning for any of these events could begin immediately and be executed within 1–2 years. The first steps are to identify volunteer organizers from the different societies who are willing to form an organizing committee, and then get approval from the staff and volunteer leadership of the relevant societies.

Task 5.4

To stimulate, coordinate, and leverage multiple stakeholders and activities, it would be valuable to catalogue and coordinate experts in MOM V&V. The first step would be to identify a champion organization or individual(s) for this task. This might include a national laboratory research group or division, a professional society committee, a university researcher group, or an industrial practitioner. Computational and experimental researchers known to be working in this area could be added to the users list, and user profiles could include categories such as academic discipline, sub-discipline, research field or interest, modeler vs. experimentalist, model length and time scales of interest, materials focus areas, etc. Either a subgroup could be developed on an existing, free platform (e.g., a LinkedIn group), or a new e-collaboration/networking platform and website could be developed. The former would be essentially free of costs, while the latter could be initiated for perhaps $10K or more, i.e., for website development or leveraging/updating an existing web site. But further funding would be required to sustain, grow, and/or market such a website/platform.

VI. Closing Remarks and Call to Action

Predictive computational models in the arena of the mechanics of materials (MOM) hold great promise for enabling significant reductions in the cost and time to develop new products and manufacturing procedures. This potential is currently constrained, however, by the inability of most models to produce trustworthy results, with quantified/quantifiable levels of accuracy and uncertainty, for product enhancement and risk management during actual production and product lifetime. In this regard, the need for rigorous model verification and validation (V&V) cannot be overestimated. Yet, efforts to consistently address this important need are currently insufficient within the relevant communities. Thus, there is a strong need to accelerate the widespread adoption and implementation of V&V activities in MOM computational modeling, such that these activities eventually become routine.

This report on the *Verification & Validation of Computational Models Associated with the Mechanics of Materials* captures and consolidates the ideas and outputs of 40 internationally recognized technical experts from a workshop held in New York City on July 27, 2018 (adjacent to the 13th World Congress on Computational Mechanics). The report presents barriers (Section III), opportunities, and recommendations (Section IV), and in-depth action plans and tasks including details such as timeframes, personnel, metrics of success, cost estimates, and potential sources of support (Section V), for accelerating the widespread implementation of V&V in MOM models. Due to the nature of V&V, the activities recommended in this report will require multidisciplinary collaboration (e.g., mechanical engineers, materials scientists and engineers, solid mechanics experts, civil engineers, designers, statisticians, computer scientists, and/or mathematicians).

Scientists, engineers, designers, policy makers and others who read this report are challenged to use the information provided here to take direct actions. Although the specific barriers, recommendations, and detailed action plans and tasks presented should not be viewed as all-inclusive, readers of this report could indeed begin to act upon many of them almost immediately, and are also challenged to use this information to learn, impart knowledge to others, and stimulate the development of additional ideas and activities that could contribute to this important cause.

More specifically, it is our desire that the readers of this report would not only find its content informative, but that many would begin addressing the action plans and recommendations outlined here by either: (a) initiating and contributing to specific research, development, and implementation efforts within their organizations, (b) providing fiscal support for such activities, and/or (3) getting involved in some of the conference, publication, and/or educational activities suggested herein. Accelerating the widespread adoption and implementation of critically needed V&V activities for predictive computational modeling in the areas of solid mechanics and materials science and engineering is critical to supporting new materials and manufacturing innovations, and the time to act is now.

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Appendix A

Full list of Barriers Identified.

*Highest priority barriers, that were presented in Section IV, are depicted here as **HP** in column 2.*

Category	Priority	Barrier
Data, Parameters, Inputs	**HP**	Limited availability of detailed, high-fidelity datasets • Relevant datasets are currently relatively sparse, making it difficult to perform accurate and robust validation
	HP	Complexity of higher dimensionality of 1) multiscale materials structures and models, 2) materials behavior mechanisms and models
	HP	Often missing fundamental understanding of underlying physics, i.e., physical conditions • Results in difficulty with calibrating parameters to compensate for missing data/mechanisms
		Lack of shared experimental data and modeling data repositories that capture metadata • Need for broad dissemination to broad MOM community
		Complexities attributed to vast number of differences among input parameters
		Quantities of interest (to predict) exceed the material- and system-level needs
		Fundamental parameters (e.g., energies, potentials) lack robust models and measurement methods
		Poor understanding of basic interactions between the parameters/inputs that drive behavior

Integrated Design of Models and Experiments	**HP**	Co-designing experiments and models is rare in the MOM community. • Researchers are often unsure how to achieve reciprocity between models and experiments; i.e., applying models (apples) versus accurate and robust validation with experiments (oranges)
		Lack of a data fusion framework to connect experiments with models • Development is largely siloed
		Non-intersecting data between experiments and models
Measurement Tools/Methods		Lack of high throughput (HT) tools to measure lower length scale responses (e.g., mechanical) • Interpretation of experimental raw data is not in a consistent framework
		Achieving statistical dependence across scales requires specialized experiments
Incentives & Resources	**HP**	Lack of motivation for providing details of V&V/UQ methods in many scientific publications (although a few publications do this) • No incentive to provide desired novel V&V insights
		Validation with UQ requires costly physical experiments and major computational processing requirements • Costs are unpredictable and/or not factored
		V&V is time-consuming • Often no clear endpoint to sufficient V&V
		Lack of hard requirements for V&V (a “stick" as opposed to a “carrot”) • No requirement incentives for V&V in MOM community (from basic science, versus engineering products)
		Verification work is often not reported because it may not be viewed by the MOM community as “exciting”, or of as much significance as the results, or the model itself
		Lack of resources • When you get to the V&V stage as it typically comes at the end of a project
Sharing/ Collaboration		Poor communication of V&V best practices/approaches
		Lack of a collaboration platform that includes V&V (e-science communities)
		Interdisciplinary 'systems' integration needed • A high degree of coupling amongst multiple disciplines

Uncertainty Quantification/ Management		Uncertainty in physical experiment • Often difficult to assess, evaluate, and capture
		Lack of UQ data extrapolation methods • Datasets for UQ are sparse • Lack of agreed-upon fundamental approaches for UQ
V&V Benchmarks and Best Practices		Lack of standardized/benchmark tests for validation as models are developed
		Sometimes too much emphasis on 'comprehensive' V&V, causing some people to avoid V&V entirely • I.e. better to at least adopt the concept that "some V&V is better than none"
		V&V for research purposes has different objectives than V&V in practice/industry
		No common/standardized methods of verification for the mechanics of materials (MOM) community to use/adopt • No mechanism for MOM community to adopt V&V practices from more V&V-proficient technical communities
		V&V typically cannot be generalized • Problems may require multiple V&V approaches
Workforce Development/ Education	**HP**	Lack of educational content and communication to build understanding of V&V/UQ in the MOM community/workforce
		[G31] Lack of a cross-disciplinary education/training (i.e., across materials, mechanics, statistics)

Appendix B

Full list of Recommendations.

*Highest priority recommendations, presented in Section V, are depicted here as **HP** in column 2.*

Opportunity Area	Priority	Recommendations
Benchmarking and Best Practices	**HP**	Create a 'best-practices' document for V&V in the MOM community • Include how to frame V&V problems
	HP	Develop a series of benchmark problems to clarify/expose good V&V practices
		Determine the 'base minimum standard' for V&V and sensitivity analyses to help raise MOM community awareness of V&V practices • Answer the question - what is the 'minimal' set of requirements for rigorous V&V?
		Build a V&V 'database' of benchmark problems for access by the MOM community
		Launch a series of benchmarking studies (i.e., similar to AM-Bench or the Sandia Fracture Challenge), but focused on 'unit tests' (i.e., not the systems level)
		Develop computational techniques/pathways (including libraries, algorithms, etc.) to conduct V&V for complex multiphysics problems

Multi-disciplinary Programs and Initiatives		Launch long-term, multi-agency-funded initiatives for dedicated V&V education across solid mechanics, materials, and statistics disciplines. • E.g., interdisciplinary research groups (IRGs) with multiple principle investigators (PIs)
		Convene remote 'e-science' working groups within the MOM community, including both experimentalists and modelers • Take advantage of existing tools within other communities
		Engage new/alternate sponsors to support MOM V&V activities
Data Repositories and Toolsets		Develop a searchable database/repository infrastructure (e.g., website) to aggregate disparate datasets across multiple sources • Requires ongoing funding commitment
		Build a dedicated repository for V&V data for MOM the community • Set metadata requirements, common formats, etc. to maximize data utility

Incentivization of V&V	**HP**	Require presentation and/or submission of V&V activities in scientific journals and other publications • Use these requirements as incentives to encourage V&V and UQ submissions
	HP	Create programs and/or a framework to help modelers and experimentalists achieve future V&V compliance requirements
		Develop research incentives, such as setting funding requirements or opportunities, to aggregate multiple compatible datasets and codes into a single source/repository • This would provide a solution for sharing/disseminating to modelers and experimentalists, for both (a) V&V teaching resources, and (b) application of V&V to specific models and problems in research and development
		Develop a means and/or culture of publishing un-validated scientific exploration models in order to stimulate new experimental work for generating new validation data
		Engage funding agencies to set V&V requirements on proposals as a way to encourage V&V implementation, as well as data sharing
		Set publication standards for metadata, experimental results, and simulation results (e.g., checklists, technical requirements, key assumptions) • Focus on making the science reproducible via proper V&V
		Use publications to incentivize code-sharing, and thus stimulate more V&V (e.g., via Elsevier Data in Brief, Journal of Open Source Software, etc.)
Sensitivity Analysis and Uncertainty Quantification	**HP**	Develop UQ methods for hierarchical (multiscale) structures and models • Develop combinatorial techniques for determining/quantifying uncertainty across length scales
		Require error bounds on both measured and modeled datasets

Making a Strong Value Proposition for V&V	**HP**	Demonstrate the value of V&V on real-life problems that are relatable to a wide range of broader society • E.g., V&V as related to industrial manufacturing of consumer products • Also communicate the negative consequences and risks of not doing V&V
		Using various communication platforms (publications, conferences, symposia) some key champions in the MOM community can help transition the perception of V&V away from being thought of as an area of interest, to a sub-discipline that should be permeating the MOM community
Workforce Development	**HP**	Create V&V courses/educational curricula • Use such courses to ultimately make V&V a commonplace technique for both modelers and experimentalists in the materials and solid mechanics communities
		Give tutorials and plenary talks about V&V at major conferences that attract MOM modelers and experimentalists • E.g., conferences for materials scientists and engineers, solid mechanics experts, mechanical engineers, the manufacturing community, etc…

TMS

The Minerals, Metals & Materials Society

Promoting the global science and engineering professions concerned with minerals, metals and materials