## **Modeling Across Scales:**

A Roadmapping Study for Connecting Materials Models and Simulations Across Length and Time Scales

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

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A Study Organized by The Minerals, Metals & Materials Society Warrendale, PA 15086

On behalf of the National Institute of Standards and Technology (NIST) Material Measurement Laboratory

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*Cover:* Representation of the three principal length scales addressed in the study: Quantum and Atomistics, Microstructural Evolution and Materials Response, and Macroscale. Three dimensional microstructure image courtesy of Dr. David Rowenhorst, Naval Research Laboratory. Cover design by Bob Demmler, TMS.

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## Contents

Acknowledgments	xi
Preface: Who Should Read This Report?	xvii
Executive Summary	xix
I. Introduction	1
II. Current State of the Art: Overview of Fundamental Materials Models, Software Tools, and Linkage Methodologies	7
A. State-of-the-Art Materials Models at Different Length Scales	8
Quantum and Atomistic Length Scale	8
Microstructural Evolution and Materials Response Length Scale.	14
Macroscopic Length Scale	
B: Some Common Software Input-Output Relationships	24
C: Current Methods and Approaches for Linking Across Length Scales	31

D: Examples of Some Current Large Scale Programs Oriented Toward Addressing Bridging Models Across Scales	. 36
III. Gaps and Limitations for Modeling Across Length and Time Scales	. 39
IV. Recommendations: Overarching Recommendations, Suggested Personnel Needed, Detailed Tactics, and Suggested Timelines	. 51
V. Closing Remarks and Call to Action	.75
VI. References	.77
VII. Appendix	. 83

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The dedication and active involvement of all of these experts has been the major foundation of this effort, and the value of their time and contributions cannot be understated. The information enclosed in this report represents the collective compilation of their efforts, and in no way represents the specific views of any of the individuals who contributed to this report, or any of their employers and/or affiliated organizations.

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## • Alexis C. Lewis: Program Director, Materials Engineering and Processing Division of Civil, Mechanical, and Manufacturing Innovation, National Science Foundation (NSF), USA

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Wing Kam Liu has made fundamental contributions to the theory and methodologies of simulation-driven science and engineering for the design of nanomaterials and the use of organic and inorganic materials for drug delivery and nano-medicine applications. He is currently president of the International Association for Computational Mechanics and chair of the U.S. National Committee on Theoretical and Applied Mechanics (TAM) within the National Academies, founding director of the NSF Summer Institute on Nano Mechanics and Materials, and co-founding director of the Northwestern Predictive Science

and Engineering Design Program. In 2014, Liu was selected as a highly cited researcher in computer science and a member of the World's Most Influential Scientific Minds by Thompson Reuters, earning him the mark of exceptional impact. Liu has earned a number of professional honors, including the 2014 Japan Society for Computational Engineering and Science Grand Prize, in recognition of outstanding contributions in the field of computational mechanics.

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- Anthony (Tony) Rollett: Professor, Materials Science and Engineering, Carnegie Mellon University (CMU), USA

Prior to joining the faculty of CMU, Anthony Rollett worked at the Los Alamos National Laboratory, where he served as a group leader and then deputy division director. His current research focuses on the measurement and computational prediction of microstructural evolution, especially in three dimensions. A 2011 TMS Fellow, Rollett's professional honors include an award for technology transfer from the Federal Laboratories Consortium (1989), the 2005 Henry Marion Howe Medal from ASM International, the 2012 Chercheur d'Excellence (Outstanding Researcher) at the University of Lorraine, Metz, France, and the 2014 TMS Cyril Stanley Smith Award. Rollett is also a co-author of the texture analysis package, popLA, and the polycrystal plasticity code, Lapp.

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Dallas Trinkle joined the faculty at the University of Illinois, Urbana-Champaign after completing his appointment as a National Research Council postdoctoral researcher at the U.S. Air Force Research Laboratory. He was named a TMS Young Leader International Scholar in 2008 and chaired the 2011 Physical Metallurgy Gordon Research Conference. His awards and honors include a 2009 NSF/CAREER award, the 2011 Xerox Award for Faculty Research at Illinois, and the 2014 AIME Robert Lansing Hardy Award. His research focuses on defects in materials using density-functional theory and novel techniques to understand problems in mechanical behavior and transport.

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# Preface: Who should read this report?

This report contains valuable information for both modelers and experimentalists within the materials science and engineering (MSE) community and for individuals from an assortment of allied disciplines from across academic, industrial, and government sectors. In addition, the gaps and recommendations identified in this study will require collaboration from this wide ranging set of communities, beyond the MSE community, in order to be adequately addressed. As discussed throughout this report, these communities may include experts within the disciplines of: mechanics, statistics, applied mathematics, signal processing, computer science, image analysis, data science and compression, software engineering, informatics, physics, chemistry, mechanical engineering, chemical engineering, and design optimization. The readers of this report can use the knowledge gained not only to learn about integration and linkage of materials models and simulations across length and time scales, but to help contribute to addressing the gaps and recommendations outlined herein. Beyond technical experts who will directly contribute to this field, readers should also include more peripherally related professionals or students who want to learn more about materials modeling across scales, or who might be engaged in guiding the enhancement of related science and technology areas.



## **Executive Summary**

#### **Motivation for this Study**

Multiscale materials modeling has been a topic of significant interest in the materials community for a number of years, largely due to the demonstrated value of robust, accurate, predictive simulations of materials behavior in greatly reducing the time and cost of developing new, advanced materials and manufacturing processes. There are many challenges, however, that must be addressed to achieve true integration and linkage of materials models and simulations across length and time scales. This encompasses the critical need for the development of fundamental linkage models, implementation strategies, quantitative computational codes, and creative new ways for engaging and convening the community. The aim of this study is to identify the current state of this field, including gaps and limitations, and provide recommendations aimed at bridging materials models and simulations across length and time scales.

#### **Study Process**

A core team was assembled to provide the bulk of the content for this study. The names, affiliations, and areas of expertise of the core team members are provided in the Acknowledgments section of this report. This team of internationally recognized experts was assembled to cover a range of materials modeling aspects, across different length and time scales, as well as a variety of different technical focus areas. They convened for a number of on-line meetings and two professionally facilitated (by Nexight, LLC), two-day, in-person meetings, and worked remotely throughout the process for the content development and the writing and editing of the final report.

Additionally, three other key volunteer teams were assembled and provided additional content development for this report (see Section I: Acknowledgements for the names and affiliations of these contributors):

- The ICME Software Team: A team of experts that met in June of 2014 for a one-day workshop near Aachen, Germany and focused on software tools employed in multiscale modeling.
- The MMM Team: A team of experts that met for a two-hour working meeting held at the site of the "7th International Conference on Multiscale Materials Modeling (MMM)" on October 6, 2014 in Berkeley, California, and focused on gaps, limitations, recommendations, and case studies involving multiscale modeling.
- The Review Team: An independent review team which provided detailed comments and recommendations on the draft of the final report for this study.

It should also be noted that in addition to materials experts, there were four mechanical engineers involved in this study (two on the core team and two on the review team). The nature of all the experts and the discussions involved resulted though in strong consideration of models of the internal structure of materials spanning the range of length and time scales (less than angstroms to meters, and picoseconds to years), with additional consideration of how these internal structures affect materials properties (e.g., the latter consideration was evident in the recommendation centered about developing strong coupling methods that allow bidirectional communication between deformation and microstructural evolution models).

The output from all of the teams and meetings described above was distilled into the final study report, which was iteratively edited by the core team, and then reviewed and edited by the review team. TMS staff then led completion of the copy editing, graphics, and production of the final report. Additionally, TMS staff organized and oversaw all aspects of this study, from inception to final report production and distribution.

#### **Current State of the Art**

An overview of some key models within given length scale regimes, analyses of some common software input-output relationships, and a review of many current state-of-the-art methods for linking across scales are presented in this report (Section II). These discussions set the stage for consideration of gaps and limitations (Section III), and recommendations (Section IV) for bridging materials models across length and time scales.

More specifically, existing materials models at the quantum and atomistic scale, microstructural evolution and materials response scale, and macroscopic scale are explored. As demonstrated schematically below for the quantum and atomistic scale, each of these length scale regimes is considered in terms of the relationships between key overarching model approaches, specific implementation approaches, and model output or property predictions.



#### **Quantum and Atomistic Length Scale**

Reproduction of Figure 2 (pg. 9): Quantum and Atomistic scale: interaction of fundamental models, implementation approaches, and property predictions.

A brief description of a number of models and implementation approaches, the current state of those models in terms of their utility and limitations, and some of the software tools available for direct implementation by the MSE community are considered in this report. A few examples include: (1) quantum and atomistic scale (pg. 9) - Quantum Monte Carlo, density functional theory, classical potentials, molecular dynamics; (2) microstructural evolution and materials response length scales (pg. 14) - crystal plasticity, phase field models, sharp interface models, discrete dislocation dynamics; (3) macroscopic length scales (pg. 20) - high strain rate modeling, solid mechanics approaches at the component level, structural system modeling, low strain rate simulations, casting and solidification models, forming models. Examples of the common software tools for community implementation of these models include: (1) atomistic scale: WIEN2K<sup>TM1</sup>, VASP<sup>TM2</sup>, Quantum Espresso<sup>TM</sup>, LAMMPS<sup>TM</sup>, ATK<sup>TM</sup>; (2) microstructural evolution and materials response length scales: Thermo-Calc<sup>TM3</sup>, ParaDis<sup>TM4</sup>, FiPy<sup>TM5</sup>, MICRESS<sup>TM</sup>, OOF<sup>TM6</sup>, MatCalc<sup>TM</sup>; (3) macroscopic length scales: Abaqus<sup>TM</sup>, Ansys<sup>TM</sup>, LS-DYNA<sup>TM</sup>, Moldflow<sup>TM</sup>, ProCast<sup>TM</sup>. A number of such relevant software tools and further details are considered in this report (Section IIB, and Section VII: Appendix).

An overview of current state-of-the-art methods and modeling approaches for bridging length and time scales is essential to providing a foundation for determining gaps and limitations (Section III) and recommendations for addressing them (Section IV). A few examples of the existing approaches for bridging length and time scales that are presented in Section IIC include: phase field crystal (PFC) modeling, density functional theory (DFT)-informed CALPHAD modeling, molecular

dynamics for dislocation mobilities, concurrent nested homogenization techniques, and multi-level finite-element methods (FE<sup>2</sup>).

#### **Gaps and Limitations**

More than 30 critical gaps and limitations that have been identified in this report for materials modeling across length and time scales are presented in Section III. These gaps and limitations stem from scientific and technical as well as programmatic issues that are hindering progress in materials modeling across scales. Section III includes details or specific examples for each gap or limitation, as well as the length scale regime(s) to which they apply, and identification as to whether they relate to concurrent or hierarchical modeling approaches. They are presented (Figure 6) in the form of a plot of relative probability of success (to overcome gaps and limitations) vs. potential impact. This summary figure from Section III is reproduced in the following. (The numbers in this plot are used as cross-references to the specific gap or limitation described in the accompanying tables in the report.)



Reproduction of Figure 6 (pg. 40): Gaps and Need Areas for Modeling Across Length Scales. Zones I-IV serve as coarse demarcations to assist the reader in following detailed descriptions in Section III.

Some of the gaps and limitations discussed in detail in Section III, and their corresponding numbers in the plot above, include: inefficiencies in existing application programming interfaces (APIs) (#2); limitations in finite-element (FE) analysis for crystal plasticity simulations (#5); the need for multiscale experiments to calibrate and validate concurrent nested homogenization approaches (#8); difficulty of determining appropriate reference values employed in CALPHAD (#10); inefficiencies of concurrent modeling with large data sets (#11); and coupling of models and experiments for performance prediction of rare events (#20).

#### **Recommendations**

The sixteen overarching recommendations (Section IV) for addressing the gaps and limitations and for making strong advances in bridging materials models across length and time scales are summarized below:

*Technical/Scientific (T):* 

- T1: Develop initiatives that address uncertainty quantification and propagation (UQ/UP) across multiple models describing a range of material length and time scales
- T2: Develop strong coupling methods that allow bidirectional communication between deformation and microstructural evolution models (i.e., methodologies to account for the co-evolution of microstructure and deformation)
- T3: Devise methods and protocols for taking into account rare events and extreme value statistical distributions
- T4: Develop multi-resolution (or multiscale) multi-physics free energy functions (and associated kinetic parameters) involving microstructure evolution, defect formation, and life prediction
- T5: Develop and execute focused research efforts addressing interfacial properties and nucleation effects, with particular emphasis on carrying out more systematic studies that couple theory, experiments, and simulations across length and time scales
- T6: Develop a multi-resolution mesoscale theory and experiments for generalized constitutive equations of evolving microstructures
- T7: Develop new, verified and validated methods to inform/derive atomic potentials
- T8: Develop predictive scaling laws and identify transitions for complex collective phenomena (i.e., emergent phenomena)
- T9: Develop methods to automatically update linkage models

#### Programmatic (P):

- P1: Establish an infrastructure for multiscale materials data
- P2: Create a network(s) for computational materials science which can help address challenges associated with multiscale modeling and simulation
- P3: Develop a set of mechanisms for increasing the coordination of international multiscale modeling efforts
- P4: Incentivize the community to develop Application Programming Interfaces (APIs) and standards for connecting different computational tools across length scales
- P5: Support open data mandates for authors to publish data in appropriate repositories as part of journal submission requirements
- P6: Convene the community to identify a large (statistically relevant), single, 4D publicly available experimental dataset to serve as the focal point of a communitywide case study in

multi-scale modeling approaches

• P7: Develop a suite of physically based analysis tools (including standard protocols for performing spatial correlations and statistics)

For each overarching recommendation the report provides an in-depth discussion, which includes: multiple tactics and guidance toward achieving the recommendations, types of personnel required, the relevant length-scale regimes addressed, and estimated time frame for completion. It is emphasized that the particular tactics suggested in this study should not be viewed as all-inclusive, and researchers, leaders, and policy makers who read this report are also challenged to use this knowledge to identify and contribute to the development of additional new tactics to accomplish the recommendations identified in the study.

Specific examples of some of the tactics, taken from two of the 16 overarching recommendations, include:

Recommendation: Develop initiatives that address uncertainty quantification and propagation (UQ/UP) across multiple models describing a range of material length and time scales.

Tactic #1:	Engage a multidisciplinary group of researchers to define terminology and
	build bridges across disciplines

- Tactic #2: Identify/define the quantities of interest at different length scales.
- Tactic #3: Define the key characteristics and forms of multiscale uncertainty
- Tactic #4: Discuss common challenges associated with UQ, and/or identify a benchmark community UQ challenge
- Tactic #5: Distinguish relevant forms of model uncertainty

## Recommendation: Convene the community to identify a large (statistically relevant), single, 4D publicly available experimental dataset to serve as the focal point of a community-wide case study in multi-scale modeling approaches.

- Tactic #1: Create a robust, experimentally measured 4D dataset.
- Tactic #2: Quantify uncertainty and verify self-consistency of the 4D dataset.
- Tactic #3: Distribute the data to modelers
- Tactic #4: Develop protocols for exchange of the data
- Tactic #5: Continually re-convene the community to evaluate and use these results

More detailed discussion for each of these tactics, and all tactics provided for the 16 overarching recommendations, are provided in Section IV.

#### **Additional Resources**

Additional resources provided in this study report include a detailed reference list, and a table of relevant materials modeling software tools including descriptions and web links (Appendix).

## **I**. Introduction

#### **Background and Motivation**

Although a number of publications and studies have discussed the value and various details of "multiscale" materials modeling (e.g., see Refs. 7–16), there remain many challenges for fundamental theoretical frameworks, methodologies, and computational codes that provide integration and linkage of materials modeling and simulation approaches across length and time scales. More specifically, bridging materials models and passing materials-related data and information across these scales is critical for the quantitative, predictive modeling needed to support the development of advanced materials and processes. As pointed out by Peter Voorhees, chair of this roadmapping study, in a recent *JOM* article:<sup>17</sup> "One of the major shortcomings with existing computational tools is the inability of a single tool to span the wide range of length and time scales that are of relevance to materials design," and "This study is focused on identifying the gaps in our ability to bridge these interfaces." As explained in the article, an important goal of the study is to provide concrete recommendations that would help address such gaps.

As an illustrative example of some specific types of linkages across length scales, classical molecular dynamics (MD) simulations can employ input from higher-resolution quantum-mechanical models such as density functional theory (DFT). For example, atomic positions and interatomic forces determined by DFT can be used to fit interatomic potentials employed in MD. The MD simulations can subsequently provide output, in the form of bulk and defect thermodynamic and kinetic properties, which can in turn be used to inform coarser scale models related to microstructural dynamics, and so on. While further development of methods for linking existing individual simulation codes is vital across scales, in many cases bottlenecks are related to the need for the development of new fundamental theoretical methodologies and frameworks for linking atomistics, microstructure,

processing, and property models across length and time scales. In other words, integration from a fundamental point of view of the physical and mathematical (numerical and analytical) approaches within the models is needed, in addition to the actual coding of linkage simulation software, at "the interfaces" between individual models, or modules. For example, beyond addressing the direct, automated flow of input/output data at these model interfaces, other more fundamental issues need to be addressed, such as uncertainty quantification and methodologies, that can make the problems tractable as one moves across length scales (e.g., homogenization techniques).

A crucial element needed for implementing such predictive models and simulations into materials design and development is their integration (note the "I" in ICME) across the productdevelopment cycle. This integration translates in part to a fundamental need for proper bridging of models across length and time scales and is an important component of the MGI "materials innovation infrastructure."

The need for and value of bridging across scales has been highlighted in the last decade by the emergence of integrated computational materials engineering (ICME)<sup>14,15,18</sup> and the U.S. Materials Genome Initiative (MGI),<sup>19,20</sup> which offer the potential to greatly reduce the time and cost of developing new, advanced materials and manufacturing process innovations. The MGI and ICME have highlighted the great value of robust and accurate predictive simulations of materials behavior. A crucial element needed for implementing such predictive models and simulations into materials design and development is their *integration* (note the "I" in ICME) across the product-development cycle. This integration translates in part to a fundamental need for proper bridging of models across length and time scales and is an important component of the MGI "materials innovation infrastructure."<sup>19</sup>

Furthermore, two recent TMS-led studies have separately pointed to the same conclusion: A critical need exists for quantitative, accurate, fundamental linkage models,<sup>a</sup> algorithms, and codes, which integrate predictive materials simulations across length and time scales. One of these studies was an internal TMS effort in which an ad hoc group of TMS volunteers focused on recommending critical materials initiatives within the core interest areas of TMS's ~12,500-strong membership. A key recommendation of this group was the development of an in-depth study with the goals of assessing current methods for integrating materials models across length scales, identifying gaps, and most importantly, identifying tactics for rapidly advancing the state of the art in this area. Within months of that recommendation, one of the outputs of the TMS study on ICME Implementation<sup>15</sup> was centered about a similar conclusion, in which it was suggested that one significant barrier to much broader implementation tools across different stages of the ICME-accelerated product development cycle (and by corollary across different length scales). As just one example, in the

a. "Linkage models" refers to models that link other models and data across length and/or time scales.

automotive industry section of the ICME implementation report,<sup>15</sup> a recommendation addresses the "Lack of Acceptable Linkage Software and Tools" and it was stated that "Although there are some available integration tools such as Isight<sup>TM</sup> and Model Center<sup>TM</sup>, smooth, efficient links between codes for processes…are still seriously lacking. This lack of versatile, user-friendly linking tools prevents the effective transmission of information between models from various length scales."

#### **Goals of This Study**

The overarching goals of this study are to: (1) provide an overview of the state of the art in materials models and related linkage models and codes; (2) identify key gaps in bridging materials models and computational tools across length and time scales; and (3) provide concrete recommendations to address these gaps and advance the state of the art in both fundamental model and implementation (code) linkages, with an emphasis on the boundaries between the fundamental models, as well as the computational tools (e.g., see Figure 1). In order to provide context for the recommendations, the state of the art in materials models and codes is first considered, followed by identification of critical gaps and limitations in multiscale modeling. Additionally, to make this study more tractable, modeling of structural materials is the particular focus.



Figure 1: Multiple length scale regimes are represented here by boxes. Bridging of these is represented schematically by arrows, but there are also finer "scale divisions," and individual models and codes, within each of the overarching length scale regimes represented here. Note: due to the significant overlap of the microstructural evolution and materials response regimes, throughout this report they will typically be treated together.

#### Process of This Study: The Volunteer Expert Teams

A lead volunteer working group, referred to hereafter as the *Modeling Across Scales* study core team, was assembled to provide the bulk of the content for this study. The names and affiliations of the core team members are shown in the Acknowledgments section of this report along with more detailed information on their areas of expertise. The core team addressed the current state of the art, gaps and limitations, and recommendations for addressing them.

This team of internationally recognized experts was assembled to cover a range of materials modeling aspects, in terms of both length and time scales, as well as a variety of different technical focus areas.<sup>17</sup> They convened for a number of online meetings and two, two-day in-person meetings, and worked remotely throughout the process for both the content development and the writing/ editing of the final report.

In addition to the core team, three other key volunteer teams were assembled and added strong value to this report (see the Acknowledgments section for the names and affiliations of these contributors):

- The review team: An independent review team which provided comments and recommendations on the draft of the final report for this study.
- The ICME software team: A team of experts that met for a one-day workshop held immediately after the 1st International Workshop on Software Solutions for ICME, which was held June 24–27, 2014 in the Netherlands, near Aachen, Germany.<sup>b</sup> This group's discussions focused on software employed in multiscale modeling.
- The MMM team: A team of experts that met for a two-hour working meeting held at the site of the 7th International Conference on Multiscale Materials Modeling (MMM) on October 6, 2014 in Berkeley, California. This group focused on gaps and limitations, recommendations, and case studies involving multiscale modeling.

Finally, it is noted that in addition to materials experts, there were four mechanical engineers involved in this study (two on the core team and two on the review team). Due to the nature of the study team expertise and how their discussions evolved though, there is a relatively strong consideration throughout this report on the internal structure of materials, spanning a range of length scales (less than angstroms to meters). Additional consideration was given to how these structures affect materials properties (e.g., in the recommendation centered about developing strong coupling methods that allow bidirectional communication between deformation and microstructural evolution models).

#### **Outputs of This Study**

This report is a roadmap for advancing the state of the art in bridging materials models and simulations across length and time scales, and includes information in the following areas:

• <u>Current State of the Art</u>: A brief discussion of the current state of the art of multiscale materials modeling, including an overview of fundamental models and software, and existing methodologies for bridging across scales (Section II).

b. web.access.rwth-aachen.de/MICRESS/ICMEg1

- <u>Gaps and Limitations</u>: Identification of more than 30 key gaps and limitations to bridging fundamental models and/or modeling tools across length and time scales. These gaps and limitations were additionally prioritized in terms of potential impact and the difficulty of overcoming them (or probability of success) (Section III).
- <u>Key Recommendations</u>: Sixteen overarching recommendations. Within each recommendation, a number of detailed tactics or sub-recommendations are provided, covering: (1) specific details to be accomplished in pursuing each recommendation (or tactic), (2) what length scales are bridged, (3) identification of the expertise (or personnel types) needed to accomplish the recommendations, and (4) the timeframe in which a recommendation (or individual tactic) might be accomplished (Section IV).
- <u>Call to action and Closing Remarks</u>: A brief summary and some guidance for next steps (and who should take them) for the recommendations of this report to be undertaken and initiated (Section V).
- <u>References/Resources</u>: (Section VI).
- <u>Existing Software Tools</u>: A table of some of the key, currently available software tools for bridging materials modeling tools across scales (Section VII: Appendix).

## Key recommendations for addressing the gaps and limitations in modeling across length and time scales

Sixteen overarching recommendations are provided. Within each, a number of detailed tactics or sub-recommendations are provided, covering: (1) specific details to be accomplished in pursuing each recommendation (or tactic), (2) what length scales are bridged, (3) identification of the expertise (or personnel types) needed to accomplish the recommendations, and (4) the timeframe in which a recommendation (or individual tactic) might be accomplished (Section VII).



## Current state of the art: overview of fundamental models, software tools, and linkage methodologies

Before considering the gaps and limitations (Section III), and recommendations (Section IV) for bridging models across length and time scales, it is important to consider what exists today in terms of individual models within given length scales regimes, as well as the current state of the art in models and codes for linking across scales. Therefore, a review of some of the prevalent models that currently exist within given length-scale regimes are presented in Section IIA, followed by some common software tool input-output relationships (Section IIB). An overview of some of the state of the art in current linkage models and codes is provided in Section IIC, followed by some examples of current large-scale programs oriented toward addressing bridging models across scales (Section IID). Although software tools are discussed throughout Section V, a consolidated table of some of the relevant software tools (including brief descriptions and web links), is provided in the Appendix.

A schematic breakdown of some overall length-scale regimes that will be referred to in this section (and in the entire report) is presented in Figure 1. It is important to note that whenever the length scale ranges depicted in the figure are referenced to methodologies, models, or codes, they should be taken to be very approximate, or relative (not literal), simply to provide some sense of reference of the applicability of the model or software being discussed. In this vein, a number of the models or codes discussed here can apply to length scales that may cross some of the ranges depicted in Figure 1.



Figure 1: Length scale regimes are represented by boxes. Bridging of these is represented schematically by arrows, but there are also many finer scale divisions, and individual models and codes, *within* each of the overarching length scale regimes represented here. Note: due to the significant overlap of the microstructural evolution and materials response regimes, throughout this report they will typically be treated together.

## A: State-of-the-Art Materials Models at Different Length Scales

This section reviews some of the prevalent materials modeling approaches that currently exist, organized within the overarching length scale regimes mentioned previously. For each of these regimes, after considering interactions among some of the associated fundamental models, implementation approaches, and outputs/property predications, brief descriptions of the individual modeling and implementation approaches are provided. These descriptions include discussion of their utility and some details of these approaches, as well as recognition of their limitations and some of the common software tools that are employed for each.

#### **Quantum and Atomistic Length Scale**

In atomistic modeling the user must balance the description of the electronic–atomistic interactions with the evolution, or optimization, of that description with the desired property prediction. Each model interaction scheme has strengths and weaknesses and implementation approaches have been developed to address equilibrium, thermally activated processes, as well as kinetics. Figure 2 provides a schematic of these relationships, and the following subsections describe in some detail the individual models and implementation approaches depicted here.



Figure 2: Quantum and atomistic scale: Interaction of fundamental models, implementation approaches, and property predictions. Note: arrows are used as a first approximation to indicate transmission of information between components of the modeling schema. Arrow colors are used to differentiate feeding of information into and out of the same implementation approach.

As represented in the schematic above, four principal modeling approaches that are commonly used as a foundation for ab initio simulations in the quantum and atomistic length scale, and describe interactions between atoms at a fundamental level, include:

- Density functional theory (DFT)
- Quantum Monte Carlo (QMC ) methods
- Classical potentials
- Ising models (including cluster expansion, lattice has)

Four key statistical or micromechanical implementation methodologies that take the outputs from the fundamental models in the first column of Figure 2 and allow quantities such as bulk thermodynamic properties and defect interactions to be calculated include:

- Kinetic Monte Carlo (KMC)
- Statistical Monte Carlo (SMC)
- Molecular dynamics (MD)
- Phonon modeling

To get a sense of how some of these different models and implementation approaches interact, the arrows in Figure 2 depict how information often flows from these fundamental models into the implementation approaches, and how the implementation approaches can lead to final property predications.

Brief descriptions of the models and implementation approaches are provided in the following, including some details of the methods and their strengths and limitations. Though the specific software tools used at this length scale can depend on the property that is being predicted, the implementation approach, or the model used to describe the fundamental interactions, common software packages for some of these models and implementation approaches are highlighted.

#### **Density Functional Theory**

Density functional theory (DFT) provides an approximate solution to the electron-ion many-body problem using the laws of quantum mechanics. Kohn and Sham<sup>21</sup> approximation methods for treating an inhomogeneous system of interacting electrons are developed. These methods are exact for systems of slowly varying or high density. For the ground state, they lead to self-consistent equations analogous to the Hartree and Hartree-Fock equations, respectively. In these equations the exchange and correlation portions of the chemical potential of a uniform electron gas appear as additional effective potentials. Significant research has gone into developing the functional and self-consistent solutions for the charge density corresponding to molecules and atoms in both solids and liquids. This provides property predictions over a wide range of chemistries with essentially no fitting parameters. One of the weaknesses of DFT is that the original formulation breaks down in regions of low electron density (vacancies, surfaces). This and other shortcomings of the original functionals have been systematically corrected over the last two decades with the introduction of the generalized gradient approximations and mixed functionals.

Although DFT is an extremely powerful modeling technique, some limitations<sup>22</sup> associated with DFT simulations are worth noting. For example, some DFT functionals predict stronger atomic bonding than what is expected from experimental observation. Additionally, DFT is limited in applications to strongly correlated materials with volumes of localized electrons (such as molecular materials and some insulating compounds). DFT is also of limited use for predicting van der Waals interactions (i.e., dispersion). However, applications to metallic systems, where the charge density is high and slowly varying, are well suited to the nature of the DFT. Also, many DFT methods employ techniques to remove tightly bound (i.e., core) electrons from the self-consistent calculations. While this approximation is valid for most chemically sensitive mechanisms, care must be taken when using these methods with the lanthanides, actinides, or in very high-pressure simulations. While electronic structure methods are very good at capturing the effects of changes in chemistry they are computationally challenging. This typically limits simulations to spatial and temporal ranges of ~1,000 atoms for less than tens of picoseconds. Over the last 10 years, embedding methods have been developed that allow simulations of defects that produce long-range elastic fields (i.e., dislocations and self-interstitials).

Despite these limitations, DFT is extremely useful and powerful for many materials design and implementation predictions, and is integral in developing simulation approaches that are built from the lowest scales up, i.e., from first principles. Such techniques are used to develop atomistic potentials to form the foundation of Ising models for thermally activated processes (kinetics), as well for studying the nature of defects as a function of chemistry.

Common software implementations for DFT include (but are not limited to) commercial codes such as VASP<sup>TM</sup> and Wien-2k<sup>TM</sup>, as well as open source codes such as NWChem, Quantum Espresso, Abinit, GPAW, and CPMD. (See the Appendix for more details on the software codes.)

#### **Quantum Monte Carlo**

Quantum Monte Carlo (QMC) is an emerging method at the quantum/atomistic length scale that could fundamentally change the way we simulate this class of problem. However, it is in a relatively early stage of development and significant progress will be required before it can be used to predict properties in complex materials. The basis of QMC involves a stochastic representation of the electronic many-body wave function. Some common challenges associated with QMC include limitations with modeling periodic systems in a scalable fashion. The computational expense is a strong limiting factor as well. More specifically, large-scale QMC calculations entail high computational expense to determine the energies associated with the system in question. Additionally, resultant force calculations require more computational effort to reduce error margins, and QMC simulations also require pseudopotentials and trial wave functions. Nevertheless, it is a technique that offers significant promise.

Although QMC codes are still by and large in the developmental stage, some that are currently available for download include QMCpack, Qwalk, and CASINO. (*See the Appendix for more details on the software codes.*)

#### **Classical Potentials**

Classical (or "interatomic") potentials attempt to represent the complex bonding interaction between atoms with significantly simpler functions that can easily be solved for energies and interatomic forces. This approach projects all the electronic structure effects (i.e., bonding) into the potential form that can mask interactions of possible interest to the final user. This is why careful and systematic testing of potentials is carried out before they are used in any simulations. While the forms of the potentials are sometimes referred to as "empirical," many of these functional forms are motivated by quantum-mechanical theories of bonding. These functions are often constructed parametrically, where the parameters are optimized to reproduce results from more accurate computation (such as DFT). The resulting potentials provide a way to extend the accuracy of DFT to larger length- and time-scales due to the computationally simpler functional forms used for classical potentials and the associated reduction in computational demands required to compute the energy and interatomic forces.

When deriving a potential for a specific system, it is important to recognize in advance what properties are ultimately to be predicted by the simulation. For example, the data input required for a melting temperature prediction will likely differ from the data needed to fit a potential for certain mechanical property simulations. Additionally, since potentials are associated with a specific material under certain conditions, transferability to other systems is often limited (e.g., an effective potential for face-centered-cubic aluminum cannot be fit to alumina systems). Therefore, since different data is used to produce the potentials, the application of the potentials should be limited to reasonably similar systems and/or condition sets. Finally, consideration should be given to how best to weight the contributions of different types of data in the development of a potential.

Software used for developing classical potentials includes codes such as Potfit and Gulp. (See the Appendix for more details on the software codes.)

#### Ising Models (Cluster Expansion, Lattice Gas)

The Lattice Gas Modeling approach is based on using an underlying lattice (Ising model) to describe the dependence of energy and other quantities on alloy system configurations. One example of this approach is the cluster expansion, where the expansion parameters are typically derived from firstprinciples techniques, and these methods utilize a lattice Hamiltonian, combined with Monte Carlo simulations, to predict thermodynamic properties. The final thermodynamic property predictions are the result of ensemble averages over multiple configurations.

A limitation of this approach is that the predictions can at best only be as accurate as the Hamiltonian value selected. In this regard, the Hamiltonian parameters become significantly more difficult to obtain as the number of chemical constituents in the simulated system increases, so the method is effectively limited to applications with fewer constituents. Additionally, the Monte Carlo ensemble approach typically assumes a fixed underlying lattice, although methods for dealing with harmonic and anharmonic atomic displacements have been developed. Overall, the lattice gas model approach is most easily applied in systems where the free energy contributions (i.e., vibrational, electronic, magnetic, configurational) are additive.

Software implementations for lattice gas modeling based approaches include a number of open source codes, such as UNCLE and ATAT<sup>23</sup>. In addition, many research groups develop their own codes for lattice gas models (and such codes are not generally available). (*See the Appendix for more details on the software codes*.)

#### **Kinetic Monte Carlo**

The Kinetic Monte Carlo (KMC) approach is typically a discrete atomistic simulation method used to model the collective, time-dependent behavior of fundamental transitions in a model system. The approach is quite general, but in the context of materials modeling it is typically used to describe either the transport of mass through a material (e.g., via vacancy diffusion) or the growth of thin films via atomic or molecular deposition. Since the application of KMC to materials modeling often involves descriptions of atomic-scale processes, the underpinnings of many KMC models are based on calculations of configurational energies using DFT. The KMC method can be employed to predict transport property coefficients for specific materials systems at given temperatures; such transport properties are often quite useful in bridging predictive materials models across scales. Since KMC is a stochastic (probability-based) calculation method, data is often acquired from the averages of many simulations in order to reduce error, and thus the computational expense can be significant despite the inherent efficiency of the underlying method. A potential limitation of KMC is its inherent inefficiency when attempting to model kinetic processes that occur at vastly different time scales (i.e., very fast and very slow events). In this case, the calculation is typically dominated by the fast event, thus "trapping" the simulation in the lower time scale. This is known as kinetic trapping, and becomes especially important when considering bridging across length and time scales.
Software implementations for KMC include SPPARKS, and an Object Kinetic Monte Carlo code developed by Los Alamos National Laboratory. (*See the Appendix for more details on the software codes.*)

# **Phonon Calculations**

The phonon calculation technique is a quantum/atomistic scale approach used to calculate basic material parameters such as thermodynamic properties. Like DFT, phonon methods are ab initio, in that they are calculated based on first principles and minimal starting conditions, but the starting points are phonons, or collections of atomic motions represented by wave vectors.

Limitations to the phonon approach arise from the harmonic or quasi-harmonic theories that underlie the approach. These theories can provide inaccurate thermodynamic properties at high homologous temperatures, or near instabilities.

Software used for phonon calculations include ATAT and PHONOPY. Algorithms for computing phonons are also implemented in some of the standard DFT codes, including VASP, Quantum Espresso and AbInit. (*See the Appendix for more details on the software codes.*)

# Molecular Dynamics (MD)

Molecular dynamics (MD) methods are used to simulate a material system as a collection of particles (typically representing atoms, ions, or molecules) that obey the laws of classical dynamics. Molecular dynamics can be used to derive bulk material properties such as the melting point, bulk and defect energies, and certain transport coefficients. With modern computational approaches MD simulations can be scaled up to simulate systems of thousands to billions of atoms, from which an array of materials properties can be predicted. The time steps are typically on the order of femtoseconds, which presents challenges related to computational expense since many time steps are required to make meaningful predictions of a number of materials properties.

One significant limitation of classical MD is that the underlying interatomic potentials do not explicitly represent important degrees of freedom such as electron exchange, magnetism, etc. The development of classical potential models that can incorporate such effects represents an ongoing active area of research (for example, in the ReaxFF (reaction force field), or bond order potential methods).

For small volumes (< 1,000 atoms) the atomic motion can be determined using DFT and the system evolved using classical dynamics. So-called ab initio molecular dynamics is used to study liquids as well as solid–liquid interfaces. Time steps are on the order of several femtoseconds and for durations of up to tens of picoseconds.

There are many commercial and open-source codes for performing classical MD simulations; common codes used for MD simulations of structural materials include LAMMPS and GULP. Ab initio molecular dynamics is available in VASP as well as other plane-wave pseudo-potential methods. (*See the Appendix for more details on the software codes.*)

# **Statistical Monte Carlo**

Statistical Monte Carlo (SMC), commonly referred to simply as Monte Carlo simulation, refers to the application of statistical-mechanics-based Monte-Carlo algorithms to compute equilibrium structural and thermodynamic properties for bulk phases and interfaces. It is a common approach for the calculation of equilibrium phase diagrams or the calculation of bulk free energies.

Statistical Monte-Carlo codes include LAMMPS, Towhee, EMC2 (part of the ATAT package), and SPPARKS. (*See the Appendix for more details on the software codes*.)



Figure 3: Microstructural evolution and materials response length scale: Interaction of fundamental properties/ parameters, implementation approaches or model types, structural data outputs, and property prediction. Note: arrows are used as a first approximation to indicate transmission of information between components of the modeling schema. Arrow colors are used only to indicate feeding of information into and out of the same implementation approach (model type).

The microstructural evolution and materials response length scale regime (which in this report refers approximately to the range from nanometers to millimeters) is the second of the three length scale regimes considered here. As depicted in Figure 3, modeling schema and information flow within

this length scale comprise a complex set of interactions between different inputs, implementation approaches, and outputs. This is due in part to the complexity of evolving microstructure, structure– property relationships, and the large number of computational materials modeling approaches available. Examples of microstructure include: grains, phases, sub-grain dislocation structures, point defect clusters, etc. Figure 3 should be thought of as an overarching representation that captures some of the basic modeling approaches towards understanding microstructural evolution and materials response (property prediction), and some of the complex interrelationships of these approaches, their inputs, and their outputs within a modeling and simulation paradigm. This figure is by no means all inclusive.

Although a number of important modeling and implementation approaches for this length-scale regime are described in the following, it should be recognized that those listed are far from a complete catalogue of the myriad techniques and tools utilized for computational materials science and multiscale modeling in this regime. The modeling approaches that are considered in some detail in this section include:

- Phase field method
- Sharp interface models
- Precipitation evolution models
- Cellular automata
- Monte Carlo Potts method
- Discrete dislocation dynamics
- Crystal plasticity
- Direct numerical simulations on statistical volume elements
- Microstructure-sensitive phase field continuum methods
- Micromechanics-based homogenization methods
- Internal state variable (ISV) models

#### **Phase Field**

The phase field method is based on evolution equations that stem from a diffuse interface model.<sup>24,25</sup> Some key advantages of this method include: there is no need to track the location of the interface explicitly, it is easy to follow interfacial topological changes, and it is straightforward to add other physical phenomena in addition to diffusion. Since the morphology of the interface is not fixed, the morphological evolution of microstructure can be conveniently determined. It is thus not surprising that this diffuse interface model has become a valuable and widely used method for simulating phase transformations.

The phase field method, like many other modeling approaches, is practically limited by the computational expense entailed in running large simulations. The challenge stems from the need to resolve a diffuse interface that has a diffuseness that is on a much smaller length scale than a typical microstructural evolution length scale. In addition, it is critical to carefully select the free energy functions for this method, since much of the accuracy of the final results rests on these functions. Some model parameters, including interface mobility or stochastic events such as nucleation, can be challenging to predict or include in the phase field method. Furthermore, the process of mapping phase field models to sharp interface models through asymptotic expansions is not always feasible.

Commonly used phase field software includes: Micress<sup>TM</sup>, FiPy<sup>TM</sup>, OpenPhase<sup>TM</sup>, and MOOSE (Marmot)<sup>TM</sup>. (*See the Appendix for more details on the software codes.*)

## **Sharp Interface Models**

Sharp interface models define a priori the topology of interfaces as surfaces (in a three-dimensional model) or lines (in two dimensions) to simulate microstructural evolution. This can be contrasted with the phase field method in which interfaces are not strictly defined at the start and are treated as diffuse in nature. Sharp interface models are widely used to model many forms of microstructural evolution, e.g., solid-state precipitate growth, two-phase coarsening, grain growth, solidification.

One challenge associated with sharp interface models is that it is necessary to explicitly track the location of the interface. In such front tracking methods, topology management must be performed explicitly, which is very difficult to implement in 3D. In addition, boundary conditions must be applied on an interface whose location must be determined as part of the solution to the problem, limiting the efficiency of some simulations. If the normal velocity of the interface can be computed, it is possible to alleviate the challenge of topology management by using the level set method.<sup>26,27</sup> Major simplifications of the sharp interface model are possible by fixing the problem geometry using appropriate material symmetries such as planar, spherical, or cylindrical. One advantage of the sharp interface model is that it is not necessary to resolve the diffuseness of the interface, which occurs on length scales that are many times smaller than the characteristic size of the microstructure.

Software used for sharp interface models includes: DICTRA<sup>TM</sup> and FiPy<sup>TM</sup>. (See the Appendix for more details on the software codes.)

# **Precipitation Evolution Models**

Precipitation evolution models for nucleation, growth and coarsening include, for example, the LSWK (Langer-Schwartz-Wagner-Kampmann) theory<sup>28</sup> for simulation of size distribution evolution. A challenge in using these models to describe these transformations is the difficulty of accurately modeling nucleation and thus a priori assumptions are typically needed. In addition, spatial correlations and diffusional interactions between precipitates are neglected in most codes. Finally, the morphology of the growing precipitates is often fixed as spherical. Precipitation evolution models are also limited in terms of the difficult-to-measure parameters needed, including: interfacial energies, nucleation parameters, dislocation densities, etc.

Precipitation evolution simulations are supported by a number of software packages including: TC-PRISMA<sup>TM</sup>, PanPrecipitation<sup>TM</sup>, MatCalc<sup>TM</sup>, and PrecipiCalc<sup>TM</sup>. (See the Appendix for more details on the software codes.)

# **Cellular Automata**

The cellular automaton approach represents a very broad class of models used for a wide variety of purposes. In the present context "cellular automata" is used to indicate modeling of microstructure by first breaking down a material into a set of cells or spaces, defining initial conditions for these cells, and then applying rules for the evolution of these cells. The evolution of these cells then progresses through multiple time steps. The method is similar in concept to the Monte Carlo Potts

model, with the primary distinction that a cellular automaton can employ any set of arbitrary rules to govern the evolution of the model system, and in particular need not conform to the procedures and requirements to which Monte Carlo methods must adhere. Computational materials scientists use the cellular automata technique to simulate microstructural evolution and similar phenomena.

A key category of limitations associated with the cellular automata approach emerges from the mathematical rules which must be imposed (for instance, rules for anisotropy of dendritic growth in solidification simulations). The rules are imposed on the cells to cause a certain geometry to emerge that approximates a physical system, but often there is not a clear underlying physics-based justification a priori for such rules. Most often, the justification is provided based on the simulation results, which is not necessarily desirable or efficient.

Software packages used for cellular automata include  $\mu$ MatIC<sup>TM</sup>, Procast<sup>TM</sup> and Sutcast<sup>TM</sup>. (See the Appendix for more details on the software codes.)

# **Monte Carlo Potts Method**

The Monte Carlo Potts method<sup>29</sup> is an approach for simulating microstructural evolution in which the evolution of each individual grain is considered in light of its local environment (with respect to grain boundaries, misorientations, etc.) and any driving forces applied to the system. The spatial distribution of the microstructure within the model domain is mapped to a pixel (in two dimensions) or voxel grid (in three dimensions). The model proceeds through many Monte Carlo time steps,<sup>30</sup> updating the identities of grid points along grain boundaries depending on the local environment, using a Monte Carlo procedure based on the definition of the system's energy (i.e. the Hamiltonian), in order to simulate microstructural evolution.

Although the Monte Carlo Potts method is a very effective technique for simulating microstructural evolution, it can be limited in its ability to capture complex physical phenomena, since the simulation is built on a simplified description of microstructural processes that does not directly address some of the fundamental, atomic-scale, diffusive processes that collectively lead to the motion and evolution of grain boundaries. Furthermore, information about anisotropies and other complex features is not typically included and often unknown in general. Finally, the computational grid or lattice imposed by the simulation can introduce various computational artifacts and errors.

Although the Monte Carlo Potts method is often supported by customized research codes developed for use at individual institutions, the SPPARKS software is an example of an open source, widely available software package for simulating not only grain growth, but also a broader class of kinetic Monte Carlo problems using massively parallel computer architectures.

# **Discrete Dislocation Dynamics**

Discrete dislocation dynamics (DDD) methods represent a material's mechanical behavior in response to external loading by calculating "the exact positions and velocities of all dislocation segments at each instant."<sup>c</sup> This is in contrast to continuum crystal plasticity models where dislocation descriptions are phenomenological and typically based on dislocation densities rather than physics-based accounting of individual dislocations. The cost of this more explicit dislocation

c. e.g., see www.dierk-raabe.com/ddd-discrete-dislocation-dynamics/

description is, of course, the relatively smaller size of the problem domain that can be efficiently investigated. Thus, DDD is quite powerful in tracking defect evolution at very specific locations of interest in the microstructure, such as the interface of a heterogeneity, grain boundary, or crack tip.

Dislocation behaviors must be described explicitly and dislocation sources must be defined accurately in order for this approach to be useful, though. Most DDD approaches have difficulty reproducing some well-known behaviors such as hardening and dislocation cell formation, particularly after large strains, and there are often challenges with representing multiphase interactions.

One common software package used to model discrete dislocation dynamics is ParaDIS<sup>TM</sup>. (See the Appendix for more details on the software codes.)

# **Crystal Plasticity**

At its core, crystal plasticity modeling relates the mechanical behavior of a crystal to slip on available slip systems. Each crystal carries with it a definition of its crystallographic orientation, such that anisotropic plastic effects can be captured through their interactions with the local mechanical state. The slip is assumed to be carried by dislocations, and crystal plasticity modeling requires knowledge of an activation stress for slip by dislocation motion, which may include dislocation-dislocation and dislocation-interface interactions, to varying extents. There are numerous ways to model behavior of polycrystals via crystal plasticity, including simplified homogenization methods (e.g., Taylor and Sachs<sup>31,32</sup>) and more sophisticated methods such as generalized self-consistent approaches. More advanced and accurate methods include finite element and finite difference approaches, with varying levels of efficiency and approximation. These techniques tend to include elastic anisotropy, unlike the standard homogenization methods. Direct numerical simulations of polycrystalline/polyphase microstructures are possible with these latter approaches, offering enhanced accuracy of local states. The state of the art in addressing the role of grain/phase boundaries in slip mediation is nascent. Crystal plasticity can be incorporated in commercial finite element method (FEM) codes, such as Abaqus, through user-defined subroutines, and emerging work on viscoplastic self-consistent codes are also being explored by some research groups.

# **Direct Numerical Simulations on Statistical Volume Elements**

This approach is based on direct numerical simulations of experimentally or simulation-derived statistical volume elements (SVEs) (or representative volume elements (RVE)) of the microstructure using the finite-element method (FEM). Key microstructural characteristics, such as the distributions of crystallographic orientation and grain size, are captured in the models using statistical measures, e.g., *n*-point probability correlations.<sup>33</sup> The use of SVEs allows a realistic representation of the microstructure while cutting down on computational expense and increasing calculation speeds, which is essential due to the increase in degrees of freedom when moving to three dimensions. Data analytics can then be used to analyze the output of the FEM simulations with respect to the 3D microstructure, for building structure–property correlations.

A disadvantage of this approach is the comprehensive collection and analysis of data from the bulk material sample (or ensemble) needed to construct statistically significant measures for appropriate SVE or RVE selection. Furthermore, while the approach is very adept at describing effective

properties and behaviors from just one weighted set of SVEs or a single RVE, a rigorous scheme has not yet been proposed to determine the statistical significance criterion for the simulation of outlier phenomena, e.g., nucleation of crack growth.

Software packages used to support this simulation approach include Zebulon<sup>™</sup>, DREAM.3D<sup>™</sup>, and DIGIMAT<sup>™</sup>. (*See the Appendix for more details on the software codes.*)

# Microstructure-Sensitive Phase Field Continuum Method

Coupling of microstructure evolution models into continuum calculations, such as the phase-field method,<sup>34,35</sup> is essentially a bridging technique contained within the overall microstructural evolution and materials response length scale regime. This approach allows basic outputs from microstructural evolution models (such as cellular automata) to be used to make more rigorous predictions about microstructure-sensitive materials behavior in which the incorporation of grain boundaries, interfaces, and other types of defects is essential.

One barrier to this approach is that the requisite phase field transformation data is often not available or is difficult to incorporate into microstructural evolution models. In other words, development of multi-physics phase field models is still in progress. In addition, standards for parameterization of such multiphysics methods (e.g., including fracture) are difficult to obtain without extensive experimental calibration, since no single free-energy equation exists to solve such coupling problems.

No known software codes are readily available for this technique.

# **Micromechanics-Based Homogenization Methods**

Micromechanics-based homogenization methods can be used for predicting the properties of a given heterogeneous microstructure. Some of the well-known methods are the Mori-Tanaka method<sup>36</sup> and self-consistent-based schemes. These methods typically are used in hierarchical multiscale modeling, where they are applied on unit cells, SVEs, or RVEs for calculating the effective properties<sup>37–39</sup> that can be passed to higher scale models.

Some software codes used for micromechanics-based homogenization methods include SwiftComp<sup>TM</sup>, Micromechanics<sup>TM</sup> LS-DYNA, and MOOSE<sup>TM</sup>. (*See the Appendix for more details on the software codes.*)

# **Internal State Variable Models**

Internal state variable (ISV) models effectively track evolution of the microstructure of a material in the context of a continuum thermodynamics approach for processes occurring away from equilibrium, simulating stress-strain-temperature behavior.<sup>40,41</sup> Such models are useful for understanding and passing structure–property relationship information across scales. Internal state variable models do not attempt to explicitly represent the complexity of the microstructure, but rather reflect averages or relatively low-order statistical moments. As is the case for any class of coarse-grained models, ISV models for a given process are not unique, and different sets or combinations of internal state variables could be applied to model evolution of the same microstructure, complicating the issue of how to pass information between scales in a hierarchical modeling scheme. However, these issues

are no different from many other coarse-grained mesoscale models. Internal state variable models can be combined with computational micromechanics, with the latter used to bridge scales. An example is crystal plasticity with slip system hardening relations that employ ISVs, along with finite element approaches for direct numerical simulation of polycrystal response.

# Macroscopic Length Scale

Modeling and simulation within the macroscopic length scale regime (i.e., roughly  $\geq 1$  mm – see Figure 1) for structural materials are heavily oriented toward processing and behavior. Different processing approaches and different behaviors entail a variety of input data types and parameters, which are sourced from a combination of experimental values and calculation outputs from simulations at lower length scales. The primary mode for taking the input data and making meaningful property predictions at the macroscopic length scale is through various finite-element (FE) codes that distill mechanical, thermal, flow/transport, and structural design information.



Figure 4: Macroscopic scale: interaction of model categories, implementation approaches, and property outputs. Note: Arrows are used as a first approximation to indicate transmission of information between components of the modeling schema. Arrow colors are used to indicate feeding of information into and out of the same implementation approach.

As represented on the left hand side of Figure 4, various modeling approaches in the macroscopic length-scale regime can, for the sake of convenience, be generally broken into two overall categories

corresponding to materials behavior and materials processing. There are many finite-element (FE) codes available for implementation of the various modeling approaches. Rather than attempting to catalogue all of them here, some of the principal modeling approaches will be considered, along with some of the relevant FE implementation codes that apply to these individual approaches (*see also the Appendix for implementation codes*).

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# High Strain Rate (e.g., Ballistics)

Component-level high strain-rate behavior modeling approaches must take into account scenarios in which materials are exposed to conditions that are quite different from the typical operating conditions of material components. One associated challenge is that high-strain-rate data can be difficult to obtain experimentally. Data needed for such simulations in the macroscopic length-scale regime include representations of substructures and joints (welds/bonds/heat-affected zones), as well as relevant failure criteria.

The timescale difference between high strain rate and low/moderate strain rates also creates a challenge. While total time scales are much smaller for high-strain-rate events, many time steps must be modeled in order to capture materials response, which means that modeling these events can be very computationally expensive.

A number of high strain-rate codes have been developed by the Department of Defense (DoD) and the Department of Energy (DOE), including ALE3D (a DOE code). Available commercial software tools for high strain rate behavior include: PAMCRASH<sup>TM</sup>, LS DYNA<sup>TM</sup>, Abaqus<sup>TM</sup>. (See the Appendix for more details on the software codes.)

#### Components

Modeling the mechanical behavior of a component (for example, a gear, a beam, or even an

individual bolt that is incorporated into a larger system) is often dependent on FE methods that are based on solid mechanics. As with all mesh-based FE approaches, the creation of the mesh can lead to errors, artifacts, or inaccuracies. While high-quality meshes have, in recent years, become easier to produce, mesh sizes and the number of degrees of freedom must still be limited in many cases to allow for reasonable computation times.

Component modeling entails a broader range of parameters beyond microstructure and basic property calculations, including factors such as contacts, interfaces, and the need to model through to component failure. Therefore, it is often computationally infeasible to retain detailed property and structural information throughout the behavior of the component, and there can be a concomitant loss of resolution (due to idealization/assumptions).

Component modeling of mechanical behavior typically relies on standard finite-element tools as well as finite-difference tools and finite strip tools for thin-walled structures. Since many of the finite element and finite strip codes are size-independent, they can be used to simulate material response in a broad range of structures, from grains to components to systems. It should be noted that, while nearly any individual size scale can be represented by an FE mesh, simultaneous representation of multiple size scales often results in large and computationally unwieldy meshes.

Numerous commercial codes (Abaqus<sup>TM</sup>, ANSYS<sup>TM</sup>, COMSOL, DYNAFLOW<sup>TM</sup>, LS-DYNA<sup>TM</sup>, NASTRAN<sup>TM</sup>) and open source software codes are available for component-level modeling, and may or may not incorporate the capability to link with computational materials approaches that address defects and microstructure. (*See the Appendix for more details on the software codes*.)

# **Structural Systems**

Structural systems refer to stand-alone, complex assemblies consisting of various components (for example, a car, a building, a plane, a bridge, etc.). Structural system modeling typically uses FEM implementations of solid and structural mechanics using collections of truss, beam, cable, plate, and/or shell elements. Models at these scales rely on average properties from experimental measurements or smaller-scale models. The idealizations and assumptions that are used to achieve a computationally feasible modeling scenario at these scales often result in loss of key details. They rely on the use of averaged, or effective, properties of materials (and sometimes even subsystems of components), making explicit modeling of fatigue, fracture, and similar properties challenging, and, in most cases, impossible when considering entire structural systems.

While many component level software tools mentioned above are also capable of modeling structural systems, a few additional software tools for systems level modeling include: OpenSees, SAP2000, STAAD.Pro<sup>TM</sup>, and Strand7<sup>TM</sup>. (*See the Appendix for more details on the software codes.*)

# Solidification

Modeling of industrial solidification processes (casting, welding, etc.) is typically reliant on multiphysics FE methods.<sup>d</sup> Input data for these simulations is quite diverse depending on the specific

d. In the present context, multiphysics refers to simulations that involve multiple physical models and/or multiple physical phenomena from different behavioral domains such as chemical, mechanical, thermal, electronic, etc.

conditions but can include: thermal conductivity and heat capacity of the material and die, heat transfer coefficients, latent heat release as a function of solid fraction, and rheological properties. A significant challenge in modeling solidification at the processing scale is the large difference in property values that occurs during the transition from liquid to solid, especially the rheology.

The macro-scale methods for modelling solidification are limited in the degree to which they can incorporate detailed information from microstructural evolution and materials response or quantum and atomistic length scales. In general, input information is limited to averaged property inputs such as those listed above. Practical limitations for multiphysics FE models of industrial solidification processes include lack of critical data needed for inputs, as well as the computational expense entailed for simulating complex geometries and local property fluctuations.

Some examples of software used for simulating casting and solidification at the macro scale include Magmasoft<sup>TM</sup>, Procast<sup>TM</sup>, SOLID Cast<sup>TM</sup>, Abaqus<sup>TM</sup>, and Sysweld<sup>TM</sup>. (See the Appendix for more details on the software codes.)

# **Deposition and Coating**

Modeling of deposition and coating processes entails thermo-mechanical considerations at both the microstructural evolution and materials response, and macro scales. Strong coupling of material flow and thermodynamics with mechanical property evolution is needed. It is not always possible to include microstructural details within these finite-element models in the macroscopic length-scale regime, either because these details are unknown or because including local microstructural information would create computationally intractable problems.

Interfaces are a significant issue in the modeling of deposition and coating processes. The largescale effects that are dictated by interfaces and interface interactions typically stem from phenomena at very fine scales. In the case of FE modeling, a common problem is the inability to represent the appropriate length scale of interfacial interactions—typically nanometers—in the same mesh as macro-scale components (millimeters and greater). While interfacial phenomena have important effects in many types of process modeling as well as microstructure evolution modeling, they are particularly pronounced in the modeling of deposition and coating processes, where a great many variables are controlled by interfacial interactions and the difference in size scales between the interfaces and the feature of interest is particularly significant.

For modeling of deposition and coating processes within the macroscopic length-scale regime, FE analysis software packages are essential tools. In addition, coupling of commercial finite element software (such as Ansys<sup>TM</sup>) with homegrown tools (such as those used to incorporate representative volume elements (RVEs)) can provide additional functionalities, such as modeling of microstructural evolution and materials response throughout the geometry of a component. As with all models at this scale, the loss of local information can contribute to errors at this length scale. The lack of input data can also be a limitation.

# Forming

Finite-element modeling of forming processes requires large amounts of input data to represent adequately the geometry and property evolution. Data inputs needed include: strength, modulus of elasticity, work-hardening behavior, anisotropy, strain-rate sensitivity, effects of temperature on mechanical properties, forming limit diagrams, fracture limit diagrams, and friction/surface properties. This entails extensive data from a combination of literature or experimental sources, or from smaller-scale calculations (particularly from microstructural evolution and materials response models).

Finite-element based software packages for modeling forming processes include: Autoform<sup>TM</sup>, LS DYNA<sup>TM</sup>, Abaqus<sup>TM</sup>, and Deform<sup>TM</sup>. (*See the Appendix for more details on the software codes.*)

## **Heat Treatment**

Finite-element modeling of heat-treatment processing at the macro scale is complicated by the fact that different models apply for different temperature ranges. For example, lower length-scale calculations that are based on moderate temperature ranges may not easily bridge into macroscale heat-treatment modeling at high temperatures. In addition, heat-treatment process models are highly contingent on the type of materials system in question, so it can be difficult to model materials that lack strong databases or literature values for data relevant to heat-treatment process–microstructure relationships.

Some common software tools for modeling heat treatment at the macroscale include: DeformHT<sup>TM</sup>, DANTE<sup>TM</sup>, and HT Tools<sup>TM</sup>. (See the Appendix for more details on the software codes.)

# B: Some Common Software Input-Output Relationships

The models described in the previous section are implemented via a variety of software, some of which are explored below. To bridge materials models across length and time scales, it is imperative to consider the data inputs and outputs of the relevant computational codes and how these data flow not only across the broader length-scale regimes considered earlier, but also between different codes within a given broad length-scale regime. Representative examples of data input-output relationships between software tools are thus shown schematically in Figure 5. This figure represents just a small sampling of materials-related software and input-output relationships in a multiscale modeling context.



Figure 5: A schematic representation of some materials modeling software tools and some common input-output relationships between them. Placement along the length scale axis should be considered to be very approximate, or relative. The dark blue boxes represent general categories of software, whereas the light blue boxes depict some specific software tools. (Note: this figure is used to indicate example input-output pathways among some common software packages, and is in no way meant to be all-inclusive.)

# Some Common Software Input-Output Relationships

More detail on the input-output data and software couplings of these tools is provided in Table 1, whereas further descriptions of the individual software tools (and their appropriate web links) are provided in the Appendix.

 Table 1: Input-Output Data and Software Couplings for Some Common Codes

CALPHAD (Calculation of Phase Diagrams) Codes (e.g., Thermo-Calc, Pandat, FactSage, Open CALPHAD)

**Input Data** for CALPHAD methods are taken from databases, including fitting parameters from which the Gibbs energies of individual phases can be calculated. The fitting parameters can be derived using several inputs.<sup>42</sup>

Input data sources include:

- Experimental Phase Diagram Data: Isothermal experiments and microstructural characterization as a function of temperature and alloy composition
- Density functional theory calculations (e.g., lattice instabilities)
- Thermochemical data represented as activity coefficients (e.g., taken from vapor pressure experiments)
- Enthalpy data

There is a large amount of experimental data available in the literature that could be used as input to CALPHAD databases, but in many cases this data is not easily accessible in an automated fashion. Data digitization efforts could yield significant value in this regard.

Difficulties can arise with inputting DFT or other computational data since the reference state of the calculation is not always clear and may not properly match the CALPHAD calculations.

**Output Data** types produced by a CALPHAD method include:

- Free energy of formation of phases (e.g., driving forces used in phase transformation models)
- Phase stability predications for microstructural evolution models
- Latent heat data to be used in solidification codes

The output data yielded by CALPHAD methods can serve as input data for a number of codes including MICRESS<sup>™</sup>, TC-PRISMA<sup>™</sup>, DICTRA<sup>™</sup>, MatCalc and ProCast<sup>™</sup>

#### **Comsol Multiphysics**

Input Data types for Comsol Multiphysics include:

- Geometric and physical outputs from computer aided design (CAD) codes
- Direct input of user field equations allowing a variety of physical phenomena to be modeled and coupled

**Output Data** types from Comsol Multiphysics include:

Numerical data, images, contour plots, and animations of multiphysics behavior at micro- to macro-scales

The output data can be used as input to higher length-scale tools

Density Functional Theory (DFT) Codes (e.g., VASP, Wien2k, NWCHEM, Abinit, CPMD, etc.)
<ul> <li>Input Data types for DFT include:</li> <li>Atomic positions (crystal/molecular structure, continuum models of defect structure, boundary conditions)</li> <li>Chemical identify of each atom</li> <li>Computation parameters (choice of basis functions, including truncation, integration parameters for reciprocal space for periodic calculations, real-space integration parameters, boundary conditions)</li> </ul>
<ul> <li>Output Data types for DFT include:</li> <li>Total energy: binding energy, transition state energies</li> <li>Derivatives of energy: force, pressure</li> <li>Optimal geometry: crystals, molecules, defects</li> <li>Defect energies</li> <li>Projected electronic density of states</li> <li>Charge density</li> <li>Electron wavefunctions</li> </ul>
The output data can be used as input to higher length-scale tools.
Finite Element Method (FEM) Codes (e.g., Abaqus, LS Dyna, Ansys, etc.)
<ul> <li>Input Data types for FEM include:</li> <li>CAD meshes or native geometry kernels</li> <li>User-defined material subroutines (UMATs), if desired</li> </ul>
<ul> <li>Output Data types from FEM include:</li> <li>RVE or component behavior in the form of contour plots, 3D animations, or tabulated results</li> </ul>
FEM codes can provide input for other tools, which are operative in the macroscopic length-scale regime. For example, Abaqus output data can provide input for Modelica™ ODE simulations.
FiPy
<ul> <li>Input Data types for FiPy include:         <ul> <li>Thermodynamic and kinetic parameters (values from CALPHAD or other databases and DFT calculations)</li> <li>Interfacial energies and mobilities (literature values taken from fitting models to experimental data, direct experimental data, or DFT calculations)</li> <li>Initial microstructures, either simulated (e.g., voronoi tessellations) or digitized experimental microstructures</li> <li>Nucleation undercooling (i.e., supersaturation)</li> <li>Thermophysical properties</li> </ul> </li> </ul>
<ul> <li>2D and 3D composition fields of phases and their morphologies</li> <li>Elastic stress and strain, temperature, and other fields</li> </ul>
Model types that could utilize FiPy output data include thermomechanical behavior models (provided adequate bridging scripts are created).

#### Material Studio Accelrys

Input Data types for Material Studio Accelrys include:

• Structure and property outputs from CAD codes

**Output Data** types from Material Studio Accelrys include:

Interactive visualizations of molecules, microstructures, surfaces, and mesoscale structures

This output data can then be used to for predicting structure-property relationships at various scales.

#### MICRESS

Input Data types for MICRESS include:

- Data from CALPHAD-based thermodynamic and kinetic databases
- Interfacial energy and its anisotropy
- Interfacial mobility
- Nucleation undercooling (supersaturation) data
- Initial conditions, and/or boundary conditions
- Thermophysical properties

Input data sources include:

- Free energies and diffusion data from CALPHAD databases
- Interfacial properties from the literature, experiments, or DFT calculations
- Initial microstructures, either simulated (e.g., voronoi tessellations) or from digitized experimentally determined microstructures

Output Data types for MICRESS include:

- 2D and 3D composition fields
- Phases and their morphologies
- Elastic stress and strain fields

Output data from MICRESS could be used in thermomechanical behavior models (utilizing custom script writing, etc.). In addition, MICRESS output data could be used for inputting to Abaqus, LS-DYNA, OOF, crystal plasticity codes, or homogenization codes. In scenarios where microstructure information is relevant, it could also be used as input to FEM codes at the macro length-scale regime.

#### Modelica

Input Data types for Modelica include:

- CAD, FEM files representing component or system structures and properties
- Experimental data can be used as input or for calibration purposes

#### Output Data types from Modelica include:

• Parametric quantities as a function of time

Modelica data can be used to produce FMI (functional mock-up interfaces) for solving complex design optimization problems.

#### Molecular Dyanamics (MD) Codes (e.g., Gromacs, LAMMPS, GULP, VMD, etc.)

#### Input Data types for MD include:

- Atomic positions and velocities
- Interatomic potentials/force fields
- Boundary conditions
- Type of dynamics (e.g., use of thermostats or barostats, rare-event sampling, thermodynamic integration)
- Time step for numerical integration of equations of motion

Output Data types for MD include:

- Atomic positions as function of integration time step (can be analyzed to yield transport coefficients and kinetic mechanisms in response to thermodynamic and mechanical driving forces)
- Ensemble averages and fluctuations for finite temperature thermodynamic properties (e.g., enthalpies, heat capacities, equations of state, stress-strain relations)
- Free energies and entropies via thermodynamic integration

Output data from MD codes can then be used as input for higher length-scale codes.

#### MOOSE

Input Data types for MOOSE includes:

- Output from CAD files
- User field equations based on the geometry in question
- Mechanical properties such as macroscopic stress and strain
- Dislocation density and dislocation spatial distribution

Output Data types from MOOSE include:

 Contour plots, 3D animations and quantitative data on of a variety of behaviors related to nuclear reactors (for example, microscopic responses of nuclear fuel to irradiation, chemicals reacting and flowing through bedrock, water and heat flow in geothermal reservoirs, etc.)

This output data is then used to support integration into higher length scale tools. Moose output data is formatted for export to third-party tools so as to support multi-scale modeling efforts.

#### 00F

#### **Input Data** types for OOF include:

- Microstructural images in common bitmap formats; such images could be sourced, for example, from microscopy or simulations (e.g., phase field)
- Constitutive parameters from the literature or prior experiments

Output Data types from OOF include:

Response fields or response functions of the macroscopic properties emerging from the microstructure, based on virtual experiments

The output data can be used as input for higher length-scale codes.

#### ParaDis

#### **Input Data** types for ParaDis include:

- Elastic constants
- Dislocation interaction data
- Nucleation data
- Appropriate boundary conditions

Input data sources include:

- Standard reference tables (experimental)
- DFT and molecular dynamics calculations

Output Data types from ParaDis include:

- Macroscopic stress and strain values
- Dislocation densities
- Dislocation spatial distributions

Output data yielded from ParaDis can be of use in software packages such as Abaqus™ or MOOSE™.

Precipitation Simulation Codes (MatCalc, PanPrecipitation, and TC-Prisma)

**Input Data** types for precipitation simulation codes include:

- Thermodynamic, molar volume, and kinetic parameters (values from CALPHAD or other databases, and/or DFT calculations)
- Interfacial energies and mobilities (literature values taken from fitting models to experimental data, direct experimental data, and/or DFT calculations)
- Average grain size (from experimental data)
- Locations for heterogeneous nucleation

Output Data types from precipitation simulation codes include:

- Precipitation Kinetics
- Particle size averages and distributions as a function of time
- Precipitate morphology evolution

This output data can be used as input data for FEM simulations of mechanical and thermal properties.

#### ProCast

Input Data types for Procast include:

- Free energies of formation for phases from software such as Thermo-Calc
- Bi-directional translators from CAD

Output Data types from ProCast includes:

• Microstructural predictions for casting simulations, stress solvers, porosity etc.

# C: Current Methods and Approaches for Linking Across Length Scales

As mentioned in the Introduction, there remain many challenges associated with fundamental models, methodologies, and computational codes that inhibit bridging of materials modeling and simulation across length and time scales. Identifying these challenges and providing recommendations for addressing them is a major goal of this study. Before considering recommendations for bridging materials models across scales, it is important to identify existing approaches and/or methodologies that are currently being (or can be) used to assist in linking materials models across length scales. Some key approaches are reviewed in Table 2 (this table is not intended to be an exhaustive compilation of all such approaches that exist). Consideration of some of these existing methods has been helpful in providing a basis to assist in identifying the current gaps and limitations in Section III, and recommendations and tactics going forward, as provided in Section IV.

For each approach listed in Table 2, in the first row just below the title of the approach/method, the <u>left hand side</u> describes the overarching length-scale regimes to which the approach applies, as referenced to Figure 1. The numbering scheme used in Table 2 for the length-scale regimes is:

- 1 quantum and atomistic scale (~ angstroms nanometers)
- 2 -microstructural evolution and materials response scale (~ 1 nm-1 mm)
- 3 the macro scale (~ $\geq$ 1 mm).

When a number range is given (such as 2–3), this is meant to indicate that the approach applies not only to potential for linkage of models *across* the length scales mentioned (e.g., 2–3), but also to linkage of different models *within* one or both of these lengths scales. As an example, the "Phase field crystal modeling" approach (first entry in Table 2), provides the potential for bridging not only *across* the quantum and atomistics through microstructural evolution and materials response scales (1-2), but also for linkage of models *within* each of these two length scale regimes (1 and/or 2). It is reiterated here that reference to these broad length-scale ranges in this context is taken to be very approximate or relative, simply to give some sense of applicability of the methodology.

The <u>right hand side</u> of the first row for each method in Table 2 suggests whether the approach applies to concurrent or hierarchical modeling (for example, the second entry, "quasicontinuum methods" applies to concurrent modeling). In the present context, concurrent modeling refers to modeling in which multiple scales operate within the same code and time step within each numerical or calculation step. Hierarchical methods refer to cases where the calculations are run independently at different length scales, and optimization methods such as statistical analysis or homogenization form the basis of communicating information between disparate scales.

There is a brief description of each approach in Table 2, along with the description of the operative length-scale regimes and concurrent vs. hierarchical nature.

#### **Table 2:** Current Approaches for Linking Across Length Scales

#### Phase field crystal (PFC) modeling

Scale Linkage regimes (see Fig. 1): 1-2 Concurrent or Hierarchical approach: Concurrent

Phase field crystal models are phase field approaches that capture processes at the atomistic scale while considering diffusive time scales. The PFC method achieves this by defining the free energy of the system in terms of classical density functional theory (DFT) with multi-resolution representation, and the method is capable of representing atomic density. Phase field crystal models can effectively describe defect evolution in response to stresses as well as thermal excitations, enabling predictions of bulk material behaviors such as solidification and melting,<sup>43,44</sup> although parameter identification is much more difficult than in traditional phase field approaches.

#### **Quasicontinuum (QC) Methods**

Scale Linkage regimes: 1-2

Concurrent

The Quasicontinuum Method (also referred to as a scale bridging method) is a modeling approach that employs the underlying interatomic potential to bridge between fully atomistic and coarse-grained regimes. When used with domain decomposition or adaptive mesh refinement, the approach is concurrent. An advantage of this concurrent scale-bridging method is that the computational expense of the atomistic calculations is drastically reduced. Adaptive refinement to full atomistic resolution is necessary to capture migration of dislocations with this method. An evaluation of this method among similar approaches is available by Miller and Tadmor.<sup>45</sup>

#### Concurrent Atomistic-Continuum Approach with FEM

Scale Linkage regimes: 1-2

Concurrent

Use of a concurrent atomistic approach with coarse-grained finite-element modeling (FEM) can either employ domain decomposition with full atomistic resolution near regions of interest (with discrete dislocation dynamics in the continuum domain), or a lattice statistical mechanics approach. Coarse and fine scales are coupled in both directions (atomistic-to-continuum and vice versa).<sup>46</sup> This kind of approach allows for passage of dislocations through the coarse-grained continuum regions.

#### Parameterized Models of Anisotropic Interface Properties

Scale Linkage regimes: 1-2

Hierarchical

Anisotropic interface properties are difficult to represent in many multiscale modeling schema, since many models (including CALPHAD) are scalar in nature. This is particularly challenging, for example, with grain boundaries where the energy of a grain boundary is a function of five degrees of freedom. Recent work, however, has made progress in reducing the degrees of freedom considerably for a given crystal system to yield an approximation for the energy as a function of misorientation and inclination.<sup>47</sup> Using this and similar parameterizations of the interfacial energy anisotropy, it is possible to incorporate these functions into multiscale models. One method for accounting for anisotropy of interface properties in hierarchical modeling schema is to utilize parameterized models employing values such as interfacial energies and diffusion coefficients as the parameters.

CALPHAD				
Scale Linkage: 1-2-3	Concurrent + Hierarchical			
The CALPHAD-based approach (originally developed for the Calculation of Phase Diagrams) is now applied to a variety of phase-based property data, including diffusion mobility, molar volume, elastic properties. It is an important length scale-bridging approach because of its versatility in accepting input data from lower length scale models, and the utility of its output data for use in higher length-scale codes, as well as its ability to extrapolate to higher component systems (frequently eight or more components) as often needed for industrial alloys. As one example of a hierarchical approach, CALPHAD outputs such as free energies of formation, latent heats, and phase stability predictions can serve as important input data for casting and solidification codes such as ProCast (bridging regimes 2 and 3)				
Density Functional Theory (DFT)-informed	I CALPHAD modeling			
Scale Linkage: 1-2	Hierarchical			
A common length-scale bridging approach <sup>48</sup> i the Gibbs free energy differences between ph (CALPHAD). This is an effective method fo evolution and materials response length scal	s to use DFT calculations of thermodynamic properties such as nases (phase stabilities) as input for phase diagram calculations r bridging from the quantum/atomistics to the microstructural e.			
DFT/CALPHAD/Phase Field				
Scale Linkage: 1-2	Hierarchical			
It is not uncommon for phase field model i extracted using the CALPHAD method. <sup>49</sup> Tak for thermodynamic and kinetic parameters ( to build a hierarchical scale bridging approact	nputs such as thermodynamic and kinetic parameters to be king into account the use of DFT approaches to provide inputs the latter through Kinetic Monte Carlo methods), it is possible th from DFT to phase field, including the use of CALPHAD. <sup>50,51</sup>			
<b>Crystal Plasticity Finite Element Methods</b>	(CPFEM)			
Scale Linkage: 1-2-3	Hierarchical			
The crystal plasticity finite-element method (CPFEM) is a scale bridging technique which combines crystal plasticity model calculations that account for crystallographic slip and lattice rotations during deformation, employing the meshing and solution methodologies of FEM, and allowing larger scales and/or specific component geometries to be considered. <sup>52</sup> This method allows for the calculation of lattice strains, anisotropic elastic response, and texture evolution in polycrystals.				
Finite-Element (FE)-Based Homogenization	on			
Scale Linkage: 2-3	Hierarchical			
Homogenization techniques facilitate estimation of effective properties or responses of often idealized heterogeneous systems (e.g., composites), including elastic behavior and evolution of microstructure (e.g. inelastic behavior). This is a powerful tool for length-scale bridging, because it can help reduce the degrees of freedom and computational expense to manageable levels for macroscale FEM. Specific methods or FE-homogenization methods include direct numerical simulation based on the concept of a representative volume element (RVE) (described in detail elsewhere <sup>53</sup> ), the generalized method of cells (GMC), <sup>54</sup> and asymptotic expansion methods. <sup>55</sup>				

Concurrent nested homogenization					
Scale Linkage: 2-3	Concurrent				
The concurrent nested homogenization approach connects two sets of homogenization data through the development of multiscale, multi-material laws. Instead of employing a single RVE to average out the microstructure information into a single material point or homogenized material property, the concurrent nested homogenization procedure involves the simultaneous (or concurrent) averaging of a selected number of different sized RVEs, all centered at the same material point so that the multi-length scale material laws can be established. <sup>56</sup>					
Multi-Resolution Continuum Theory (MCT	)				
Scale Linkage: 2-3	Concurrent				
Traditional continuum mechanics theories entail characterizing the neighborhoods of the particular material points in the simulation via their primary degrees of freedom (DOF). <sup>57</sup> On the other hand, multi-resolution continuum theory (MCT) techniques take into account not only the primary DOFs but also append additional DOFs to describe each material point in terms of its neighboring conditions, in an attempt to more accuratel simulate complex behavior. <sup>58</sup> Such techniques are important for achieving higher levels of sophistication in developing structure–property relationships. <sup>59</sup> Multi-resolution continuum theory is centered on applying the nonlocal and strain-gradient descriptions to multiple length- and strain-rate scales, respectively, thus regularizing the strain over each of the scales to predict local and non-local deformations, fracture patterns, and ultimate failure of material components Multi-resolution continuum theory does not provide an explicit separate scale description of the material, i.e. the microstructure is neither explicitly modeled nor is it concurrently coupled with the macro-scale. Whe compared to the concurrent multiscale modeling methods (e.g. the "guasicontinuum method" summarized i					
Multi-Level Finite-Element Method (FE <sup>2</sup> )					
Scale Linkage: 2-3	Concurrent + Hierarchical				
For some systems, multi-level finite-element methods can be used to effectively model macroscale or component level behavior, while concurrently taking into account microstructure damage evolution. This method employs an FE computation of the system's representative volume element concurrently with component-level FE analysis, allowing the larger-scale simulation to incorporate rigorous microstructural evolution information. <sup>60</sup> One software system known to support such functionalities is Abaqus <sup>™</sup> .					
Projection-Based Reduced Order Approac	ch				
Scale Linkage: 2-3	Concurrent				
A common challenge for multiscale modeling of realistic microstructures is the computational expense incurred for high-fidelity models. In order to make applicable modeling across length-scale problems more tractable (both mathematically and computationally), projection-based reduced-order methods can be employed to reduce the degrees of freedom, while retaining an acceptable level of fidelity. Mathematical techniques can be employed to reduce the degrees of freedom, or the problem can be approached from a data-driven perspective, via data compression or by reducing the data analyzed to a smaller set of principal components, eliminating less important features via intelligent sampling. <sup>61</sup>					

Multiphysics free energy representations				
Scale Linkage: 2-3	Concurrent			
Most free-energy representations are developed based on a single physical problem or scenario, for example, the study of phase transformations in materials or the study of fracture mechanics via a phase-field representation. A multiphysics free-energy representation entails developing a single free-energy representation to study more complex, interacting phenomena, such as the effect of phase transformations on fracture, or the effect of fracture on phase transformations. Multiphysics free-energy representations could more effectively encapsulate complex problems and interactions, which could then in turn be used in concert with higher length-scale simulations. This approach allows more complex scenarios to be modeled within a multiscale approach. <sup>62</sup>				
Analytical/Semi-Analytical Micromechani	cal Approaches			
Scale Linkage: 2-3	Hierarchical			
Analytical or semi-analytical approaches often complement or augment direct numerical simulations, particularly for capturing homogenized properties and their dependence on microstructure. These approaches can be based on analytical solutions such as the Eshelby Inclusion analysis for a particle in a matrix, <sup>63</sup> which provides stresses, strains, and mechanical energies in the material, and can be generalized to multiple inclusions. These approaches can also be based on rigorous bounds for properties (i.e., limits that are independent of specific microstructure) such as the Hashin–Shtrikmann bounds; <sup>64</sup> higher-order bounds and approximate estimates are also available. Such approaches can apply to mechanical, thermal, electrical, and transport properties of complex materials, and additionally include the rule of mixtures (for stiffness components) and the Mori–Tanaka method <sup>36</sup>				
Commercial Systems Integration Codes f	or Linking Multiple Codes/Tools			
Scale Linkage: 1-2-3	Concurrent + Hierarchical			
An important enabling toolset category for effective multiscale modeling is codes that link together multiple modeling codes. In particular, tools that allow for scripting of the transfer of the output of one code into another code as input are helpful for configuring and executing hierarchical modeling schema. Some commercial examples of such integrative modeling environments include ModelCenter <sup>™</sup> , iSight <sup>™</sup> and Simulia <sup>™</sup> , and the Academy Materiale Studie <sup>™</sup> .				

the Accelrys Materials Studio™.

# **D:** Examples of Some Current Large Scale Programs Oriented Toward Addressing Bridging Models Across Scales

In addition to considering the current state of the art of specific models at various length scales (Section IIA) and linkage models and codes (Section IIC), some examples of broad, multi-researcher projects that are currently beginning to address bridging materials models across length and time scales will be considered here. This is by no means intended to be an all-inclusive survey, but instead is meant to provide some current examples.

One such project, supported by the U.S. Department of Energy – Energy Efficiency and Renewable Energy Office program, applies an ICME methodology to develop advanced steels for automotive applications. In particular, this project "ICME Approach to Development of Lightweight, Third-Generation Advanced High-Strength Steels" is aimed towards the development of a suite of integrated models to predict properties of third-generation advanced high-strength steels (3GAHSS) with an eventual goal of using this suite for integrated design purposes<sup>e</sup> This program is being executed through the United States Automotive Materials Partnership LLC (USAMP—a collaborative organization of Chrysler Group LLC, Ford Motor Company, and General Motors), in collaboration with the Auto/Steel Partnership (A/SP), based on a DOE-EERE award of \$6 million over four years (supplemented by \$2M in matching funds). Phase I of the project focuses on model development and validation, and integrates results from existing computational and experimental methodologies, spanning numerous length scales, to develop a suite of models to predict the properties of 3GAHSS, while phase II focuses on integration and design.<sup>f</sup>

A number of major efforts related to multiscale modeling have been initiated as a result of the Materials Genome Initiative (MGI), with a particular emphasis toward development of the MGI materials innovation infrastructure. For instance, the PRISMS program (PRedictive Integrated Structural Materials Science), which is centered at University of Michigan (UM), is supported by the Department of Energy (DOE) – Basic Energy Science offices as part of their MGI efforts.<sup>g</sup> The primary goal of the PRISMS program is to develop an integrated suite of validated computational tools to accelerate structural metals design. Some PRISMS objectives that specifically relate to modeling across length and time scales include: establishing an integrated multi-scale modeling

f. see www.uscar.org/guest/news/666/Press-Release-USAMP-RECEIVES-6-MILLION-AWARD-FROM-DOE-FOR-ADVANCED-HIGH-STRENGTH-STEEL-PROJECT; http://www.autosteel.org/~/media/Files/Autosteel/ Great%20Designs%20in%20Steel/GDIS%202013/The%20Next%20Generation%20of%20Advanced%20 High-Strength%20Steels.pdf for details

g. prisms.engin.umich.edu/

e. see www.uscar.org/guest/news/666/Press-Release-USAMP-RECEIVES-6-MILLION-AWARD-FROM-DOE-FOR-ADVANCED-HIGH-STRENGTH-STEEL-PROJECT; www.autosteel.org/~/media/Files/Autosteel/ Great%20Designs%20in%20Steel/GDIS%202013/The%20Next%20Generation%20of%20Advanced%20 High-Strength%20Steels.pdf for details

framework and open source software; developing advanced open source computational methods; tightly coupling experiments and models for application and validation; and establishing the "Materials Commons"—an open source knowledge repository and virtual collaboration platform. More specifically, the PRISMS Center is organized around four topics: precipitate evolution, recrystallization and grain growth, tensile behavior, and fatigue behavior of magnesium alloys. These topics serve as demonstrations and test beds for the capabilities of the PRISMS framework.

Also under MGI, the National Institute of Standards and Technology (NIST) is supporting (\$25M over five years) the Center for Hierarchical Materials Design (CHiMaD), a Chicago-based consortium that includes Northwestern University as the lead, the University of Chicago, and Argonne National Laboratory.<sup>h</sup> ChiMaD is focused on developing computational tools, databases and experimental techniques that will enable the accelerated design of novel materials and their integration into industry. In relation to modeling across length scales, CHiMaD aims to focus its approach on the creation of novel hierarchical materials, which exploits distinct structural details at various scales. Specific goals along these lines include: foster hierarchical materials discovery by developing next generation of prediction, measurement, and interpretation; connect and convene current experts and the next generation of scientists through multi-disciplinary and multi-sector communication via workshops, seminars, training opportunities, and meetings; and serve (with NIST) as a national resource for verified codes and curated databases.

Two other MGI-related programs, both centered at Johns Hopkins University (JHU), include the U.S. Air Force Center of Excellence on Integrated Materials Modeling (CEIMM),<sup>i</sup> and the U.S. Army-sponsored Materials in Extreme Dynamic Environments (MEDE) Collaborative Research Alliance (CRA).<sup>j</sup> The Center of Excellence on Integrated Materials Modeling entails a multiinstitution research and education consortium, which includes members from academia, the air force laboratories, and industry, to foster advances in computational and experimental methodologies supporting the theme of integrated computational materials science and engineering (ICMSE), and using approaches that are applicable to a variety of materials. Three guiding principles behind the CEIMM approach include: innovations in theoretical, computational, and experimental methods; integration across scales, disciplines, materials classes, processing, and performance; and multidisciplinary education to support the new generation of engineering workforce. In terms of modeling across scales, the CEIMM program combines modeling and experiments through integration of physics-based multiscale models, multiscale characterization and virtual models, multiscale experimental methods, and uncertainly quantification. Materials in Extreme Dynamic Environments is also a collaborative research program that includes JHU, the U.S. Army Research Laboratory, California Institute of Technology, Rutgers University, and the University of Delaware. The MEDE approach is both multiscale and multidisciplinary and includes canonical modeling, experiments to identify mechanisms, modeling, and simulation at different length and time-scales (and scale bridging), integrated models or codes, and integrative experiments with multiscale diagnostics and robust datasets.

h. chimad.northwestern.edu/

i. ceimm.jhu.edu/

j. See www.arl.army.mil/www/pages/1419/1419\_MEDE Overview.pdf

The Consortium for Advanced Simulation of Light Water Reactors (CASL)<sup>k</sup> is a DOE Energy Innovation Hub led by Oak Ridge National Laboratory (ORNL), and provides advanced modeling and simulation solutions for commercial nuclear reactors. The Consortium for Advanced Simulation of Light Water Reactors' six technical focus areas include advanced modeling applications, physics integration, radiation transport methods, materials performance optimization, validation and uncertainty qualification, and thermal hydraulics methods-all using an interdisciplinary collaborative approach to develop and apply their Virtual Environment for Reactor Applications (VERA). Of interest concerning materials modeling across length and time scales, the components in VERA simulate nuclear reactor physical phenomena using coupled multiphysics models, and VERA includes the software development environment and computational infrastructure for these components. Another large nuclear-energy based DOE program involving materials modeling at different scales is the Nuclear Energy Advanced Modeling and Simulation (NEAMS) program, supported by the DOE – Nuclear Energy office.<sup>1</sup>An overarching NEAMS goal is to gain new insights into the performance and safety of nuclear energy technologies by developing tools for modeling and simulation. For example, in the fuels product line (FPL) portion of NEAMS, there is a focus on developing predictive computational capabilities for multiscale fuel performance simulation, covering length scales from atomistics to mesoscale to fuel performance models, using the NEAMS Pellet-to-Plant Simulation Toolkit.

The programs discussed here were provided as a few examples of large-scale, government-supported projects that are currently beginning to address bridging materials models across length and time scales, and the reader of this report is referred to some relevant web links as a starting point to learn more about these programs. This subsection is not meant to be an all-inclusive summary of such projects, but instead is meant to provide some current examples. It is also hoped that researchers from such programs will find value in the gaps and limitations (Section III), and the recommendations (Section IV) provided in this report to help guide their efforts to maximum effect for the broader modeling across length and time scales community.

k. www.casl.gov/

I. See https://inlportal.inl.gov/portal/server.pt/gateway/PTARGS\_0\_2\_156611\_0\_0\_18/FY15\_NEAMS-1.pdf

# Gaps and Limitations for Modeling Across Length and Time Scales

In addition to considering the current state of the art in modeling approaches at given length scales (Sections IIA and IIB) and exploring current methods for scale bridging (Section IIC), some key gaps in bridging materials modeling capabilities across length and time scales have been identified. These areas should be addressed by the community in order to advance the state of the art in scale bridging techniques. In Figure 6, these gaps and limitations have been roughly organized based on the degree of potential impact in addressing them, as well as the estimated relative probability of successfully overcoming them. The number values in the plot in Figure 6 have no special significance, rather they are used to cross-reference to the specific gaps or limitations described in Tables 3A–3D. The four quadrants in Figure 6 provide general guidance for this rough prioritization scheme of the gaps and limitations, as follows:

- **Quadrant I**: Higher Impact, Higher Probability of Success These gaps and limitations can be thought of as low-hanging fruit for near-term efforts.
- **Quadrant II**: Lower Impact, Higher Probability of Success These gaps and limitations can also be thought of as low hanging fruit, but of lower priority, given their lower estimated projected impact.
- **Quadrant III**: Lower Impact, Lower Probability of Success These areas represent lower priorities identified, but would still be helpful for the field if addressed.
- **Quadrant IV**: Higher Impact, Lower Probability of Success These areas can be thought of as some of the larger challenges facing the community. Though they will be challenging to address, they promise significant impact if achieved.

The boundaries between the quadrants in Figure 6 should not be viewed as discreet lines of demarcation, but instead as "diffuse" borders which help with coarse level differentiation or grouping of the gaps and limitations.

The corresponding tables (Tables 3A–3D) provide details on the specific gaps and limitations depicted in Figure 6. The two columns on the right hand side of Tables 3A–3D address the same approximate length scale regimes (via the numbering scheme) and hierarchical (H) vs. concurrent (C) modeling category used in the two columns of Table 2 in Section IIC—these numbering and category schemes are defined just above Table 2.



Figure 6: Gaps and Limitations for Modeling Across Scales

Many of the simulations performed as part of a multiscale modeling schema entail significant computational expense. Computational expense becomes intractable when scaling up from lower length and time scales to make meaningful predictions at higher scales. Although techniques are used or being developed for more efficient bridging strategies, an increase in available computing power to a broader user base would also be of significant value to the multiscale modeling community.

Table 3A (Quadrant I): Higher Impact, Higher Probability of Success – Gaps and Limitations				
#	Title Description	Scale	Туре	
1	Barriers to Reduced Order Models Reduced order modeling is an essential tool for reducing the degrees of freedom (e.g., the number of elements in a finite-element simulation) so as to increase computational efficiency and make larger scale problems tractable. However, there are a number of barriers to effective reduced order modeling. For example, it is unclear what the minimum number of data sets or points for accurate prediction is in a given modeling schema. Models are needed for intelligent sampling of data sets to help increase efficiency (fewer data points equates to better computational efficiency) while retaining accuracy. Principal Component Analysis is an example of a reduced order approach, but more work is needed in this area.	2-3	C+H (Concurrent & Hierarchical)	
2	<ul> <li>Inefficient Application Program Interfaces (APIs)</li> <li>Programming interfaces between many codes are either not readily available, or are inefficient.</li> <li>Some specific examples include: <ul> <li>Phase field calculations are not rapid when linking to CALPHAD via existing APIs. For phase field simulation, free energy minimization is sometimes needed within the model.</li> <li>Ideally, Gibbs energy minimization code should be written directly inside a fracture code for instance, and should then interface with CALPHAD.</li> </ul> </li> <li>There are many linkage scenarios in which APIs have not been developed at all.</li> </ul>	2-3	C+H	

3	Propagation of Damage: Scaling from Localization to Effective Properties When modeling damage of materials (such as ductile failure) one major multiscale challenge is scaling up from the local microstructural phenomena, such as void formation or dislocations, to the final, effective property, such as component failure or other higher scale damage.	2-3	Н
4	<ul> <li>Insufficient Number of Open Data Repositories</li> <li>Experimental and computational data needs to be more accessible to facilitate wider adoption of multiscale modeling approaches.</li> <li>Some specific needs for stimulating the sharing of data include:         <ul> <li>Incentive models for the materials community to share data and tools</li> <li>Strategies for encouraging "open science" or "reproducible science" in the materials community</li> <li>Common data standards for both experimental and virtual data to improve interoperability</li> </ul> </li> </ul>	1-2-3	C+H
5	Finite-Element (FE) Analysis for Crystal Plasticity – Computational Efficiency FE analysis for crystal plasticity-based microstructure simulations is computationally intensive to an extent that it limits the practical use of this method for guiding materials development. Methods are needed to improve efficiencies of such calculations to improve the utility of this approach.	1-2	С
6	Limited Computing Power Many of the simulations performed as part of a multiscale modeling schema entail significant computational expense. Computational expense becomes intractable when scaling up from lower length and time scales to make meaningful predictions at higher scales. Although techniques are used or being developed for more efficient bridging strategies, an increase in available computing power to a broader user base would also be of significant value to the multiscale modeling community.	1-2-3	C+H
7	<b>Discretization at Disparate Length and Time Scales</b> Materials structure and behavior are often described using discretization methods such as FEM where a specific grid size and time interval are employed (making the modes discrete in terms of length and time). A major challenge to employing such methods at multiple length scales is that the different scales require different grid densities and time steps, creating difficulties in passing information up to higher scales.	2-3	Н

8	Multiscale Experiments Needed for Concurrent Nested Homogenization In order for concurrent nested multiscale modeling approaches (homogenization) to be effectively realized, multiscale constitutive equations (laws) are needed which will require true multiscale experiments to calibrate the equations, as well as effective methods of simplified parameterization.	2-3	С
9	Barriers to Concurrent Modeling of Atomistics and FEM Domain Size Limits When using concurrent methods to bridge from atomistic approaches up to finite element modeling, domain size is limited by computational expense, causing a loss in resolution and failure of some critical information to propagate to higher scales. Boundary Conditions Boundary conditions can dictate that defects emerging at the atomistic length scale cannot propagate further unless the propagation can be accounted for at the atomistic scale as well. This is a limitation in the underlying physics, rather than the linkages themselves.	1-3	С

# Table 3B (Quadrant II): Lower Impact, Higher Probability of Success - Gaps and Limitations

#	Title Description	Scale	Туре
10	<b>Difficulties in Determining Appropriate Reference</b> <b>Values Employed in CALPHAD</b> For example, when using DFT end-member reference values such as free energies of formation or lattice stabilities in CALPHAD databases, it is a challenge to identify the appropriate reference values to use. These difficulties emerge from multiple sources. For instance, the DFT reference points for pure components may not match up to literature values for standard reference stabilities (e.g., see Ref. 65), in part due to the "Zero-Kelvin" problem, namely that DFT is calculated at zero Kelvin and then adjustments are needed to estimate values at temperatures relevant to the phase diagram. In other cases, where complex systems are calculated based upon simpler systems (for example, if the phase diagram of an ABCD system is developed based on the AC system and the BD system), emergent phases that are not present in the simpler systems will lack DFT predicted end-member values. Adoption of standards for reference values would help facilitate linking of different methods.	1-2	H (Hierarchical)

11	Inefficiencies of Concurrent Modeling with Large Datasets When coupling via concurrent multiscale methods, large datasets increase computational expense to an impractical degree. An example of this is that phase field modeling coupled with CALPHAD becomes too slow when using full databases. Techniques are needed to work around this limitation, such as improved adaptive sampling or other methods for reduced order modeling.	1-2	С
12	<b>General Computational Limitations for Finite-</b> <b>Element Analysis</b> Finite-element analysis (FEA) is computationally limited in its ability to represent and model all the relevant data in components or systems from multiple scales. For instance, modeling grain geometries and boundaries of interest for simulations in the 100–1,000 grain range at multiple scales with good resolution would entail very high computational expense. Idealizations and assumptions are needed to make calculations tractable, which leads to resolution losses.	1-2-3	C+H

# Table 3C (Quadrant III): Lower Impact, Lower Probability of Success - Gaps and Limitations

#	Title Description	Scale	Туре
13	<b>Uncertainty in Multi-Component CALPHAD</b> It is difficult to predict uncertainty in multicomponent CALPHAD simulations. Addressing this would represent a step forward in building towards uncertainty quantification for multiscale modeling approaches.	2-3	C+H (Concurrent & Hierarchical)
14	Diffusivity Simulations do not Account for Second Order Effects Diffusion by the vacancy method can be modeled as the movement of solute atoms or as the movement of vacancies. As vacancies move, there are effects on the energy barriers of neighboring atoms as well as on second nearest and third nearest neighbors; however, most analytical diffusion simulations only take into account the nearest neighbors. This can lead to appreciable error in these simulations, which can then propagate when bridging scales.	1-2	Н

15	Lack of Anisotropy in Models As a primary example, CALPHAD calculations are scalar in nature, primarily focused on calculating the free energy of formation of phases under certain thermodynamic conditions. A major limitation of CALPHAD models is that they do not account for more complex, anisotropic conditions that can ultimately affect the free energies of formation. For example, anisotropic strain due to lattice conditions could modify the energy for precipitate formation. Similarly, interfacial energies that differ depending on facet geometry or anisotropic diffusion are phenomena that would not be effectively captured by CALPHAD. These effects all have significant impact on linking across scales during materials modeling, since CALPHAD is so instrumental in many scale bridging scenarios. Similar problems associated with lack of information on anisotropy exist in other approaches as well.	1-2	C+H
16	Kinetic Trapping of Kinetic Monte Carlo (KMC) Simulations A challenge associated with the KMC method is known as kinetic trapping. This challenge arises when modeling physical scenarios in which higher scale phenomena arise from lower scale events that occur at very fast time steps. The calculation can essentially become "trapped" at the lower, faster scale without a mechanism to effectively simulate the higher scale phenomena.	1-2	Н
17	<b>Non-Uniqueness for Inverse Problems</b> Inverse modeling methods can be used to gain insights into mechanisms or starting conditions via downscaling, back calculations or interpolation methods, but a significant challenge is accounting for non-uniqueness when moving from the observed low-dimensional space to the underlying high-dimensional space. Specifically, there are many scenarios where multiple mechanisms or starting condition combinations could feasibly lead to the same results. This is a significant source of uncertainty in inverse problems.	2-3	Н

A wide ranging problem for modeling and simulation of structural materials is accurately identifying the microstructural features that are critical to property evolution, in particular at the higher length- scale component and system level.

Tab	le 3D (Quadrant IV): Higher Impact, Lower Probability of Sur	ccess – Gaps a	nd Limitations
#	Title Description	Scale	Туре
18	<b>Barriers to Multi-Level Finite-Element Methods (FE</b> <sup>2</sup> ) Multi-level FE methods can be a powerful approach for bridging length scales, since the technique allows FE analysis of critical features at multiple length scales. However, when using such methods, it is not computationally feasible to analyze every feature at the lower scales, and the end results will be heavily dependent on which features are selected, so this selection process can be a significant challenge. Use of representative volume elements and other statistical methods to represent the lower-level length scales can help, but does not eliminate the challenge entirely. In addition, better validation experiments are needed to demonstrate whether multi-level finite element methods for defect propagation etc. are valid for scenarios such as high strain rate problems.	2-3	C (Concurrent)
19	<b>Identifying Critical Microstructural Features</b> A wide ranging problem for modeling and simulation of structural materials is accurately identifying the microstructural features that are critical to property evolution, in particular at the higher length- scale component and system level.	2-3	C+H
20	Performance Controlled by Rare Events – Lack of Adequate Coupling of Predictive Models and Experiments Where performance is controlled by rare events that are often not tractable from an experimental stand-point (e.g., in fatigue), coupling of models and experiments to predict performance is extremely challenging. This is especially an issue when scaling up, for instance, from microstructure and defects to properties and final component or platform performance.	2-3	Н
21	<b>Limitations of Periodic Boundary Conditions</b> In simulated microstructures, periodic boundary conditions are often employed. This assumption can limit the accuracy of the overall simulated microstructure and resulting property predictions (at higher scales).	2-3	С
22	<b>Need for Better Pre-Conditioners</b> A wide ranging need for multiscale modeling approaches to improve, is the need for better mathematical "pre-conditioners," i.e., mathematical techniques that condition a given problem into a form that is more suitable for solution by numerical methods.	1-2-3	C+H

23	Handling of Multiple Scales That Can Exist within the Microstructural Evolution and Materials Response Level Microstructures are generally complex, and rather than being treated at one length scale, in reality can have many smaller, relevant length scales depending upon the materials system. Being able to treat scales within the multitude of different materials systems in a consistent fashion would be helpful in terms of simplifying modeling approaches, but is currently a major challenge. One example of multiple scales within a given microstructure is the phenomena of a "twine within twine"	2	Н
24	Addressing Uncertainty Quantification and Propagation Across Scales The need to adequately address uncertainty quantification and propagation (UQ/UP) is critical yet typically not adequately addressed in a multiscale context, particularly in the mechanics of materials communities. Uncertainty quantification has been addressed for some modeling approaches at individual scales, but propagating the uncertainty across scales is very challenging. This is the case primarily because UQ is typically handled differently at different length or time scales even down to the conceptual level. In addition, in situations where it is feasible to pass uncertainty values up from a lower scale to a higher scale, it is not always clear how to understand these values or what practical insights can be made from them. Getting communities that have strengths in this area, particularly the statistics and probabilistic methods communities, involved with materials modeling efforts is a key step towards solving this problem. Overall, more dialogue between researchers with disparate skillsets is needed in order to address this grand challenge.	1-2-3	C+H

Getting communities that have strengths in this area (UQ/ UP), particularly the statistics and probabilistic methods communities, involved with materials modeling efforts is a key step towards solving this problem. Overall, more dialogue between researchers with disparate skillsets is needed in order to address this grand challenge.

25	<ul> <li>Verification and Validation (V&amp;V) Needs</li> <li>Validation of models needs to be conducted in a rigorous statistical framework that accurately accounts for uncertainties in experimental measurements at various length and time scales. In addition, ensuring that the experimental information contains all relevant data for validation of models is critical. For example, minor impurities in the experimental samples, unaccounted for in the metadata, could introduce significant error in the validation process, which then propagates across scales during multiscale modeling.</li> <li>More readily available experimental data on alloys and other materials (in shared databases, repositories, etc.) would help contribute to V&amp;V of models at different scales becoming common practice.</li> <li>Common standards for data originating from experiments and simulations would help ease the comparison process needed for model validation at all scales.</li> <li>Establishing consistent, agreed-upon protocols and ranking criteria for reliability of a given model (i.e., model maturity or model readiness level) will be an essential step for the community for robust V&amp;V of these models (narticularly as they are bridged across scales)</li> </ul>	1-2-3	C+H
26	<b>Difficulties with Linking Dislocation Dynamics with</b> <b>Continuum FEM Models</b> Dislocation dynamics methods are intrinsically difficult to link to continuum FEM methods, such as standard crystal plasticity methods. Mesh free methods or extended finite-element modeling (XFEM) methods need to be employed to greater effect to address this linkage challenge.	2-3	С
27	<b>Immaturity of Interface-Mediated Crystal Plasticity</b> Crystal plasticity calculations are based on FEM scenarios where the grains are deformed. A limitation to current crystal plasticity approaches is that they do not typically account adequately for interfaces. This can affect modeling over a range of length scales, as well as model bridging between the microstructure evolution and materials response, and macroscale regimes.	2-3	С
28	<ul> <li>Timescale Mismatch Between Length Scales <ul> <li>A key challenge to some multiscale modeling and simulation scenarios is that there is a timescale mismatch over different length scales for dynamic problems.</li> <li>Examples <ul> <li>In modeling of crack propagation, multiple time scales are operative. At the crack tip, the atomic vibrations and their associated time scale is of significance, whereas for the rest of the crack, the dynamics are best described at higher time scales.</li> <li>In modeling particle nucleation and growth, the nucleation events occur in picosecond ranges, whereas the full precipitation can evolve in seconds to hours. This could refer to for example, aging precipitates in aluminum agehardened alloys, carbide precipitation in steels, etc.</li> <li>Fatigue is difficult to model because of time scale mismatch. The cyclic loading events are at one time scale (perhaps seconds) whereas the ultimate failure can occur in the timescale of years.</li> </ul> </li> </ul></li></ul>	1-2-3	C+H
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29	<b>Difficulty of Determining Interfacial Energies</b> Multiscale phase transformations simulations are limited by the difficulty of obtaining accurate interfacial energies (particularly by experimental techniques).	2	н
30	Inability to Account for Emergent (Unpredicted) Phenomena A fundamental limitation to modeling of materials systems, and particularly multiscale modeling, is the inability to account for emergent behavior using domain driven design efforts. "Emergent phenomena" in this context refers to behavior that emerges, often unexpectedly or unexplainably, from interactions at a lower scale. In particular, higher length scale models are often not tailored to effectively capture emergent phenomena (such as the formation of dislocation cell walls) that can nonetheless be critical contributing factors to property evolution.	1-2-3	C+H

31	<b>Missing Underlying Physics in Materials Models</b> One of the biggest challenges (and opportunities for growth) lies in the fact that although some large strides have been made in the development of multiscale modeling and simulation approaches in recent years, there are still significant limitations and gaps in the individual modeling capabilities that serve as the foundation for modeling across length and time scales. These limitations in materials modeling are often due to failures of the model to properly incorporate the underlying physical mechanisms that drive behavior or the materials parameters needed to make the models quantitative	1-2-3	C+H
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## IV. Recommendations: Overarching Recommendations, Suggested Personnel Needed, Detailed Tactics, and Suggested Timelines

A number of recommendations have been identified toward addressing the gaps and limitations explored in section III, and toward making strong advances in modeling across length and time scales. Tables 4A and 4B below provide a summary of the overarching recommendations and corresponding tactics, which detail possible pathways for realizing the recommendations' goals. The recommendations are split into two categories: those which are deemed technical/scientific ("T" – Table 4A), and those that are considered to be more programmatic in nature ("P" – Table 4B). Although all of the recommendations were deemed important, within each category below (technical – Table 4A, vs. programmatic – Table 4B), the recommendations have been prioritized, ordered from those deemed the highest priority items at the top (lower numbers) and the relative priority of the recommendations decreasing down the list (higher numbers).

Following the tables is a detailed discussion of the recommendations and their corresponding tactics. This includes suggestions for the types of personnel or expertise required to pursue these recommendations, as well as comments on the relevant length scale regimes to which the recommendations apply. For each of the sixteen overarching recommendations, specific tactics are provided and discussed, and time frames are suggested for when they might be achieved. The time frames are roughly categorized here as either short (corresponding to approximately three years or less), medium (3–5 years), or long (5–10 years).

It must be emphasized that throughout this report the specific tactics presented should in no way be viewed as all-inclusive, and researchers, leaders, and policy makers who read this report should also feel challenged to contribute to the development of additional new tactics to accomplish the overarching recommendations identified here.

#### Table 4A: Technical/Scientific Recommendations

<u>Recommendation T1</u>: Develop initiatives that address uncertainty quantification and propagation (UQ/UP) across multiple models describing a range of material length and time scales

- <u>Tactic #1</u>: Engage a multidisciplinary group of researchers to define terminology and build bridges across disciplines
- Tactic #2: Identify/define the quantities of interest at different length scales
- <u>Tactic #3</u>: Define the key characteristics and forms of multiscale uncertainty
- <u>Tactic #4</u>: Identify common challenges associated with UQ, and/or identify a benchmark community UQ challenge
- <u>Tactic #5</u>: Distinguish relevant forms of model uncertainty

<u>Recommendation T2</u>: Develop strong coupling methods that allow bidirectional communication between deformation and microstructural evolution models (i.e., methodologies to account for the co-evolution of microstructure and deformation)

- Tactic #1: Incentivize collaboration across the mechanics and materials communities
- <u>Tactic #2</u>: Identify key experimental data sets for verification and validation (V&V) of such coupling models
- Tactic #3: Develop computationally efficient paradigms (models and tools) for such coupling

### <u>Recommendation T3</u>: Devise methods and protocols for taking into account rare events and extreme value statistical distributions

- <u>Tactic #1</u>: Develop computational and experimental approaches and techniques to explore detection of special features and events
- <u>Tactic #2</u>: Develop experiments to support validation of models which account for rare events and extreme value statistics
- <u>Tactic #3</u>: Develop a new computational paradigm that accounts for rare events and extreme value statistical distributions
- <u>Tactic #4</u>: Establish strong collaborations amongst materials scientists, signal processing experts, statisticians, and computer scientists to develop methods to detect rare events

<u>Recommendation T4</u>: Develop multi-resolution (or multiscale) multi-physics free energy functions (and associated kinetic parameters) involving microstructure evolution, defect formation, and life prediction

- <u>Tactic #1</u>: Incentivize collaborations of experts in the materials science and engineering community who will address this problem
- <u>Tactic #2</u>: Develop the strategies for constructing coupled multi-physics free energy functions
- <u>Tactic #3</u>: Distinguish separation of length and time scales of the schema for these treatments
- <u>Tactic #4</u>: Develop strategies for handling "far from equilibrium" conditions

## <u>Recommendation T5</u>: Develop and execute focused research efforts addressing interfacial properties and nucleation effects, with particular emphasis on carrying out more systematic studies that couple theory, experiments, and simulations across length and time scales

- <u>Tactic #1</u>: Develop more efficient, robust, high-throughput experimental approaches to measure interfacial free energies
- <u>Tactic #2</u>: Integrate experimental approaches and theory through incentivized collaboration among groups doing experiments, modeling, and theory
- <u>Tactic #3</u>: Canvas existing best practices for scale-bridging strategies
- <u>Tactic #4</u>: Develop new scale-bridging strategies involving nucleation and interfacial phenomena

### <u>Recommendation T6</u>: Develop a multi-resolution mesoscale theory and experiments for generalized constitutive equations of evolving microstructures

- <u>Tactic #1</u>: Incentivize collaborations
- <u>Tactic #2</u>: Nanoscale to microscale bridging
- <u>Tactic #3</u>: Microscale to mesoscale bridging
- Tactic #4: Integration of results from tactics #2 and #3

#### <u>Recommendation T7</u>: Develop new, verified and validated methods to inform/derive atomic potentials

- <u>Tactic #1</u>: Develop best practices, new algorithms, and standardized codes for fitting interatomic potential models and for assessing their transferability
- Tactic #2: Approach issues of validation and uncertainty quantification (UQ) in an efficient manner
- <u>Tactic #3</u>: Develop good practices for sharing and checking of potentials

### <u>Recommendation T8</u>: Develop predictive scaling laws and identify transitions for complex collective phenomena; i.e., emergent phenomena

- <u>Tactic #1</u>: Hold workshops
- <u>Tactic #2</u>: Validate low-order physical interactions in predictive scaling laws
- Tactic #3: Develop automated approaches to extract scaling laws from arbitrary (small) simulations

#### <u>Recommendation T9</u>: Develop methods to automatically update linkage models

- <u>Tactic #1</u>: Establish various community linkages for specific problems
- <u>Tactic #2</u>: Interface APIs and data infrastructure
- <u>Tactic #3</u>: Consider these methods during new/evolving model development
- <u>Tactic #4</u>: Create robust, adaptive tools that are materials-domain agnostic
- <u>Tactic #5</u>: Develop reduced-order models for smart sampling across scales

#### **Table 4B:** Programmatic Recommendations

#### Recommendation P1: Establish an infrastructure for multiscale materials data

- Tactic #1: Engage other communities with experience in this area for lessons learned
- <u>Tactic #2</u>: Explore commercial routes for establishing such an infrastructure of federated databases
- <u>Tactic #3</u>: Work with various agencies to facilitate establishment of a database network

### <u>Recommendation P2</u>: Create a network(s) for computational materials science that can help address challenges associated with multiscale modeling and simulation

- Tactic #1: Create the network or individual institutes
- <u>Tactic #2</u>: Convene workshops, symposia, and/or conferences
- <u>Tactic #3</u>: Address curriculum recommendations and development
- <u>Tactic #4</u>: Develop short courses

### <u>Recommendation P3</u>: Develop a set of mechanisms for increasing the coordination of international multiscale modeling efforts

- Tactic #1: Convene international expert panels to develop roadmaps and encourage networking
- Tactic #2: Convene multiscale modeling researchers virtually
- Tactic #3: Create research funding opportunities jointly between multiple nations
- <u>Tactic #4</u>: Define a set of Foundational Engineering Problems to be pursued by the global modeling and simulation community

### <u>Recommendation P4</u>: Incentivize the community to develop Application Programming Interfaces (APIs) and standards for connecting different computational tools across length scales

- <u>Tactic #1</u>: Convene groups of experts to identify state-of-the-art API technologies and available computational materials codes
- <u>Tactic #2</u>: Incentivize API development through Small Business Innovation Research (SBIR) programs (industry) and specific research programs (academia and national laboratories)
- <u>Tactic #3</u>: Develop data translators and information passing protocols (for input-outputs)
- <u>Tactic #4</u>: Establish standards for materials data representation
- Tactic #5: Establish connections between materials science and computer science faculty and students

### <u>Recommendation P5</u>: Support open data mandates for authors to publish data in appropriate repositories as part of journal submission requirements

- <u>Tactic #1</u>: Develop solutions for large data transfer and storage
- <u>Tactic #2</u>: Develop metadata descriptions
- Tactic #3: Develop standards and methodologies for publishing data provenance
- <u>Tactic #4</u>: Develop new incentives for data sharing

<u>Recommendation P6</u>: Convene the community to identify a large (statistically relevant), single, 4D publicly available experimental dataset to serve as the focal point of a community-wide case study in multiscale modeling approaches

- Tactic #1: Create a robust experimentally measured 4D dataset
- <u>Tactic #2</u>: Quantify uncertainty and verify self-consistency of the 4D dataset
- <u>Tactic #3</u>: Distribute the data to modelers
- <u>Tactic #4</u>: Develop protocols for exchange of the data
- Tactic #5: Continually re-convene the community to evaluate and use these results

<u>Recommendation P7</u>: Develop a suite of physically based analysis tools (including standard protocols for performing spatial correlations and statistics)

- <u>Tactic #1</u>: Data analysis tools for high-throughput methods
- <u>Tactic #2</u>: Community analysis tools based on reduced-order methods

#### **Technical/Scientific Recommendations**

### <u>Recommendation T1</u>: Develop initiatives that address uncertainty quantification and propagation (UQ/UP) across multiple models describing a range of material length and time scales.

This recommendation is best addressed by experts in the fields of materials science and engineering, mechanics, statistics, and applied mathematics, as well as researchers who make contact with related uncertainty quantification and propagation (UQ/UP) issues in other disciplines (e.g., mechanical engineering, chemical engineering, etc.). This recommendation applies to bridging efforts across all length scale regimes (angstroms to meters).

### <u>Tactic #1</u>: Engage a multidisciplinary group of researchers to define terminology and build bridges across disciplines

A common language or nomenclature for addressing UQ/UP issues is needed across materials science and engineering, mathematics, computer science, statistics, and other UQ/UP communities in order to facilitate collaboration and expertise-sharing across discipline domains. Significant progress should be achievable on this front in the near term.

#### Tactic #2: Identify/define the quantities of interest at different length scales

It is imperative to determine the quantities of interest at different length scales for which it is most critical to quantify and track uncertainty, particularly as these parameters are passed between models and across length and time scales. This area requires development since consideration of uncertainty for discrete modeling approaches that distinguish between model and parameter uncertainties are not well developed. This could be addressed by either individual researchers or groups working together on collaborative research projects, in a medium term time frame.

#### Tactic #3: Define the key characteristics and forms of multiscale uncertainty

In the medium term this would encompass defining the *forms of uncertainty* at different scales, as related to the quantities of most interest (see tactic #2). In the long term, this would involve defining the critical characteristics of *how uncertainly propagates* across length and time scales through transitions among disparate models, relative to both the most relevant quantities being considered and the different forms of uncertainty.

### <u>Tactic #4</u>: Identify common challenges associated with UQ, and/or identify a benchmark community UQ challenge

This tactic is best addressed by experts across the fields of materials science and engineering, mechanics, statistics, and applied mathematics working together, and could involve workshops, conferences, and/or special issues or sections in journals, conference proceedings, and books. Significant progress on this tactic should be feasible in the short term.

#### Tactic #5: Distinguish relevant forms of model uncertainty

Both epistemic (reducible) and aleatory (irreducible) forms of uncertainty are significant for model forms and parameters, as well as for multiscale model linking strategies. Conventional Gaussian forms for probability distribution may not be sufficient for addressing uncertainty in the context of discrete modeling environments such as density functional theory and molecular dynamics, when model degrees of freedom are limited/quantized. Since uncertainty quantification and propagation for such cases and for linking schemes is not presently well developed, progress is needed and is expected to be feasible in the medium to long term.

# <u>Recommendation T2</u>: Develop strong coupling methods that allow bidirectional communication between deformation and microstructure evolution models (i.e., methodologies to account for the co-evolution of microstructure and deformation)

This recommendation applies to microstructure evolution models for cases of thermal exposure (e.g., coarsening, grain growth, precipitation), where the resultant microstructures can then feed back into relevant deformation models. It also applies for the effects of dislocation substructure formation or damage evolution within microstructures at large deformation or fracture/fatigue failure conditions. In other words, co-evolution methodologies for microstructure evolution and deformation are required. These could, for instance, encompass an iterative scheme in which microstructure evolution simulations are performed for representative volume elements (RVEs), with resulting property evolution and structure fed back into the deformation models, which then update the microstructural models, and so on. Although there are many microstructure evolution models (for instance for Oswald ripening,<sup>66–69</sup> nucleation,<sup>70–72</sup> precipitate growth,<sup>72–74</sup> and overall precipitation,<sup>28</sup> as well as deformation and/or damage models,<sup>57,75–77</sup> much work is yet to be done in quantitative coupling of such microstructure evolution and deformation/damage models. This recommendation would best be addressed by researchers from the materials science and engineering, mechanics of materials, and computational science communities.

#### Tactic #1: Incentivize collaboration across the mechanics and materials communities

Creating incentives for the mechanics and materials communities to approach this challenge collaboratively entails a short term tactic (3 years or less). Specifically, such incentives should aim to bring appropriate experts from these communities together to identify the key areas of need for such coupling, and to roadmap specific solutions in this arena. Methods to execute this tactic could include glue grants<sup>m</sup>, workshops, symposia, specialty conferences, and special, targeted publications or journal feature issues.

### <u>Tactic #2</u>: Identify key experimental data sets and associated computational tools for verification and validation (V&V) of such coupling models

This would be a short term tactic (3 years or less) to identify and collect existing methods, models and codes. This would involve identifying existing data sets that could be leveraged for V&V of the coupling/linking models, as well as determining the key types of data sets that would be required, and then working with relevant experimentalists to develop new data sets in this arena. This tactic could also be leveraged with recommendation P6, below.

m. Glue grants refer to grants that specifically support collaboration and interactions among researchers (e.g., meeting, travel, etc.) on individual projects supported by other sources, in cases when such integration adds value to an overarching goal.

Tactic #3: Develop computationally efficient paradigms (models and tools) for such coupling This would be at least a medium term endeavor (3–5 years), and perhaps longer term. By leveraging Tactics #1 and #2 above, this would involve researchers working together in a concerted way to develop creative new schemes, methodologies, algorithms, and implementation codes, to couple specific microstructure evolution and deformation models and codes. This would likely involve new projects focused solely on this goal, including, for instance, individual Ph.D. theses, as well as larger collaborative efforts involving multiple research groups working together on different facets of the same goal. Some generic examples of such past or current larger collaborative efforts associated with various science and technology goals include the Office of Naval Research/Defense Advanced Research Projects Agency (DARPA) D 3-D program, the DARPA Accelerated Insertion of Materials (AIM) program, the National Institute of Standards and Technology (NIST)-sponsored ChiMaD (Center for Hierarchical Materials Design) center of excellence,<sup>n</sup> and the Department of Energy (DOE)-sponsored PRISM (PRedictive Integrated Structural Materials Science) program.<sup>o</sup>

More specifically, such coupling efforts could be approached in a number of ways. Direct Application Programming Interface (API) codes could be developed that are focused on passing microstructural data back and forth between microstructural evolution model implementations such as phase field codes (e.g., MICRESS<sup>TM</sup>, FiPy<sup>TM</sup>, OpenPhase<sup>TM</sup>) and various deformation modeling codes (e.g., Deform<sup>TM</sup> Autoform<sup>TM</sup>, LS DYNA<sup>TM</sup>, Abaqus<sup>TM</sup>)<sup>p</sup> (see the Appendix for a more complete list of existing codes). This sub-tactic on APIs also dovetails directly with recommendation P4 below.

In addition to APIs for direct transmission of data across codes (input and output), new paradigms and coupling methods are also needed, which could include new theoretical and mathematical frameworks. Promising work along these lines for integrating phase field method and Thermo-Calc databases has been suggested.<sup>78</sup> It could also include integrating microstructure evolution models associated with thermal exposure and deformation modeling at a higher level, before the actual implementation within publicly available computational tools, such that the models could exist and communicate within a single implementation/integration platform.

### <u>Recommendation T3</u>: Devise methods and protocols for taking into account rare events and extreme value statistical distributions

To address this recommendation, materials science and engineering researchers should work with the signal processing community (for feature detection), statistics experts (for generalizing extreme value statistical problems), and the computer science community. This recommendation may best apply in the nm-to-mm length scale regime.

### <u>Tactic #1</u>: Develop computational and experimental approaches and techniques to explore detection of special features and events

The materials science and engineering community should take advantage of the strong expertise and existing algorithms and computational tools already developed by the signal processing community.

p. Although there are some available APIs including those within integration tools such as Isight<sup>™</sup> and Model Center<sup>™</sup>, APIs between many/most of the existing microstructure evolution and deformation codes are still not available.

n. chimad.northwestern.edu/

o. prisms.engin.umich.edu/#/prisms

It is expected that this recommendation might be able to be adequately addressed and implemented in the medium term (3–5 years).

### <u>Tactic #2</u>: Develop experiments to support validation of models which account for rare events and extreme value statistics

This effort would be paced not only by the creative thinking and ability of researchers to develop and set up such experiments, but by innovations of companies/vendors who are constantly enhancing and developing new capabilities of equipment for materials characterization and testing. It is expected that significant development and implementation of such experimental methodologies might be achievable in the medium (3–5 years) time frame.

### <u>Tactic #3</u>: Develop a new computational paradigm that accounts for rare events and extreme value statistical distributions

Developing a new computational paradigm for this problem would entail a long term effort, and would likely require sustained collaborations and integration of experts amongst the materials science and engineering, signal processing, statistics, and computer science communities (see also tactic #4 below). A concerted effort from a wide variety of experts would be needed in order to devise new methodologies, algorithms, implementation codes, and experimental validation techniques that adequately address rare events and extreme values in an efficient and integrated manor, and bridge length and time scales.

### <u>Tactic #4</u>: *Establish strong collaborations amongst materials scientists, signal processing experts, statisticians, and computer scientists to develop methods to detect rare events*

Establishing cross-community collaborations amongst materials scientists, signal processing experts, statisticians, and computer scientists could involve some of the same techniques described under recommendation T2, Tactic #1 above; namely: (1) glue grants, (2) workshops, (3) conferences, and (4) special issues or sections in journals, conference proceedings, or books. Another potential approach would be the co-advising of graduate students on joint projects by professors collaborating across the relevant departments within universities. These activities could be undertaken in the short term (three years or less).

# <u>Recommendation T4</u>: Develop multi-resolution (or multiscale) multi-physics free energy functions (and associated kinetic parameters) involving microstructure evolution, defect formation, and life prediction

This recommendation addresses strategies for constructing free energy functions to support coupled multi-physics modeling. Execution of this recommendation will require an umbrella of basic research efforts encompassing scientific theory, computational approaches ranging from DFT to mesoscale phase field approaches, and validation experiments. This recommendation pertains to length scales ranging from approximately angstroms to tens of microns and time scales from picoseconds to seconds, and dovetails in different ways with recommendations T6, P6 and P7. Tactic #1 below could be executed in the short term, and would help set the foundation for addressing this recommendation, while tactics #2 through #4 outline more specific approaches that would likely be achievable in the longer term (5–10 years).

### <u>Tactic #1</u>: Incentivize collaborations of experts in the science and engineering communities who will address this problem

This would be a short term tactic (3 years or less) aimed at bringing appropriate experts together to identify the key types of multi-resolution, multi-physics free energy functions needed, coming up with specific strategies for their development, and forming teams to work together on this effort. Mechanisms for executing this tactic could include workshops, symposia, and/or glue grants.

<u>Tactic #2</u>: Develop the strategies for constructing coupled multi-physics free energy functions Develop strategies to compute and incorporate various relevant contributions of free energy into multi-physics functionals. This includes entropic contributions as appropriate for different materials classes and applications.

#### Tactic #3: Distinguish separation of length and time scales of the schema for these treatments

The challenge is handling different characteristic length and time scales that do not easily separate. The coarse-graining of the free energy functionals with scale is a critical issue in moving from first principles at nanoscales to more complex mesoscales and cooperative kinetic mechanisms for microstructure evolution (e.g., Ginzburg-Landau<sup>79</sup> and Cahn-Hilliard<sup>24</sup> equations of phase field theory).

#### Tactic #4: Develop strategies for handling "far from equilibrium" conditions

Development of such multi-resolution (or multiscale) multi-physics free energy functions will be challenging in and of itself; developing and applying such functions in a fashion which adequately addresses physical phenomena associated with conditions that are far from equilibrium will present another set of challenges, and is likely a longer term endeavor.

One of the most challenging areas of multiscale materials modeling involves addressing interfacial properties and nucleation effects in an accurate, quantitative way, and properly linking this information across length and time scales.

<u>Recommendation T5</u>: Develop and execute focused research efforts addressing interfacial properties and nucleation effects, with particular emphasis on carrying out more systematic studies that couple theory, experiments, and simulations across length and time scales.

To be adequately addressed, this recommendation would require input from personnel with a variety of expertise areas including modelers, experimentalists, and theorists in the materials science and engineering (MSE) community. In particular, this recommendation could be addressed by researchers with expertise in the design of experiments, interfacial energy/properties measurements, and crystallographic metrology. Additionally, modelers and experimentalists with working knowledge in modeling areas including, but not limited to, phase field simulations, atomistics, density functional theory (DFT), and continuum mechanics would add great value. Although this

recommendation could apply to multiple length scale couplings (e.g., the outputs from such work could apply from angstroms to meters), this recommendation would be especially applicable in the angstrom-to-50 nm length-scale range

One of the most challenging areas of multiscale materials modeling involves addressing interfacial properties and nucleation effects in an accurate, quantitative way, and properly linking this information across length and time scales. For instance, although there have been a plethora of excellent studies on solid state nucleation (e.g., see Refs. 70–72), it is well known that quantitative nucleation modeling (for a variety of materials) still presents many challenges, owing in part to the difficulties associated with making accurate measurements of critical nuclei and nucleation rates to serve as input data for direct validation of the models across different materials systems.

Another significant, related challenge in modeling across scales is the dearth of direct measurements of interfacial properties, particularly interfacial energy,<sup>q</sup> which is critical to many forms of modeling, including those centered about nucleation. For instance, for nucleation of simple geometries (such as spheres), the cube (third power) of the interfacial energy ( $\gamma$ ) lies within the exponential of a term in the nucleation rate equation; thus, very small differences in the interfacial energy can make very large (orders of magnitude) differences in the calculated nucleation rate.<sup>70,72</sup> Interfacial energy is also a critical parameter in the modeling of Oswald ripening (both two phase coarsening and single-phase grain growth), precipitate strengthening, precipitate growth, crack nucleation and propagation, fracture, fatigue, and other key properties.

It is thus recommended that more concerted efforts be made on (a) enhancing the quantification, and validation of nucleation theory and simulations, (b) the accurate quantitative determination of interfacial energies across a wide range of materials systems and interface types (including solid:solid, solid:liquid, and solid:vapor interfaces) and, most importantly, (c) bridging the nucleation modeling and interfacial properties across scales (length and time). To achieve this overarching recommendation, four specific tactics for making progress in this area are identified below. (It is re-emphasized that these are not all-inclusive solutions, and readers of this report are challenged to develop other creative ways to address recommendation T5.)

### <u>Tactic #1</u>: Develop more efficient, robust, high-throughput experimental approaches to measure interfacial free energies

Current methodologies for measuring interfacial free energies typically have either one of two shortcomings: they are indirect and/or they are very consuming. Indirect methods include for example techniques to back-calculate interfacial energies from coarsening experiments coupled with theory, such that these values are dependent on the assumptions, details, and execution of the models themselves. Other methods, such as zero creep, thermal grooving experiments prove to be very time consuming. Experimentalists are challenged to develop and employ creative methodologies to obtain direct measurements of interfacial energies in an efficient manor, so that they can be applied as input to (or validation of) simulations over a larger range of materials systems and applications, and length and time scales. Potential experimental approaches for meeting this challenge could involve combinatorial analyses, or more widespread use and continued development of 3D techniques which sample large numbers of grains or precipitates and their crystallography, inclination, and

q. In this context "interfacial energy" and "interfacial properties" refer to any form of interface; e.g., solid:solid, solid:liquid, or solid:vapor interfaces

interface groove angles (e.g., Refs. 80,81). Although some progress can be made in this area in the short or medium term, it is estimated that development of new, very high throughput experimental techniques for measuring interfacial energies over a wide range of materials systems or conditions is a long-term proposition.

It is also recommended that experimental researchers share such interfacial energy values obtained via these techniques with the broader community, especially modelers, through publication and other methods of data sharing. It is crucial that the researchers developing this type of data interact intimately with appropriate modelers, not only after they obtain the data, *but before they do the experiments as well*, so that they can gain insight into the specific types of interfacial energies that are most relevant to the models. It is equally important for experimentalists to identify for modelers the materials systems and applications that are most critically in need of predictive modeling involving interfacial energies. This integration of modeling and experimental efforts will help accelerate materials-related innovations and implementation of materials solution involving this type of data. This feedback loop of communication between experimentalists and modelers should be continuous and interactive, and is the subject of the next tactic.

### <u>Tactic #2</u>: Integrate experimental approaches and theory through incentivized collaboration among groups doing experiments, modeling, and theory

Progress in the area of nucleation modeling, interfacial energies, and bridging nucleation modeling and interfacial properties across length and time scales will not be achieved in any robust fashion or reasonable time frame without the close collaboration of experimentalists and modelers, focusing on more direct integration of experimental and modeling approaches. As just one example of this type of integrated approach, image-based modeling<sup>82</sup> (also referred to as microstructure-based modeling<sup>83</sup>) is a promising methodology to pursue, in which experimentally determined microstructures (preferably in 3D) and their interfaces and interface properties are used as direct input for simulations. For example, measured 3D microstructures and microstructural parameters have been used as direct inputs for FE models simulating microstructure response to externally imposed stress fields,<sup>82,84</sup> as well as for phase field simulations of microstructure response to thermal loads.<sup>6,85</sup> However, a much broader degree of integration of experimental approaches and simulations is needed across the MSE and related communities, involving a plethora of models, experimental methodologies, and length and time scales.

Methods for incentivizing such collaborative interactions and integration between experimentally focused researchers and modelers include glue grants, workshops, conferences, and publications such as special issues or sections in journals, conference proceedings, and/or books. Workshops and conferences could be facilitated by the engagement of materials related professional societies, while targeted publications could be developed in coordination with journal or book editors and publishers, as well as professional societies (for journals managed by a professional society). These types of activities should be undertaken in the short term (3 years or less).

#### Tactic #3: Canvas existing best practices for scale-bridging strategies

Although cataloguing of some of the existing linkage models in the state-of-the-art section near the beginning of this report is an initial step toward this specific recommendation, more detailed benchmarking which explicitly identifies best practices associated with detailed methodologies would be of great value. This could be achieved perhaps with the aid of a workshop or study involving multiple researchers in the field, or possibly under the guidance of broader stakeholders in this area (e.g., a consortium or project addressing modeling at different length and time scales). This type of investigation should be achievable in the short term.

<u>Tactic #4</u>: Develop new scale-bridging strategies involving nucleation and interfacial phenomena Developing new scale-bridging strategies for nucleation and interfacial phenomena is a much broader recommendation than some of the other tactics and thus would be a long term proposition. Some directions in which to begin might include using existing multi-resolution approaches as a foundation from which to focus on bridging nucleation modeling and interfacial properties across scales, as well as using such concepts as input for phase field simulations during consideration of both microscopic and macroscopic degrees of freedom.

### <u>Recommendation T6</u>: Develop a multi-resolution mesoscale theory and experiments for generalized constitutive equations of evolving microstructures

This effort would involve researchers over effectively the entire spectrum of the MSE community as well as other communities such as computer science, mathematics, statistics, signal processing, and others. An overarching end goal for this recommendation would be the development of a theoretical and computational framework, linked to experiments, for bridging microstructure evolution models across a range of scales (from nanometers to millimeters), via constitutive equations. Execution of this full recommendation would involve a long-term commitment; although various tactics toward execution could be completed in shorter timeframes (see below). This recommendation dovetails in various ways with recommendations T4, P6, and P7.

#### Tactic #1: Incentivize collaborations

Incentivizing such collaborations would be a short term tactic (3 years or less) to help get this effort off the ground by stimulating collaborations amongst the broad spectrum of modelers and experimentalists required to achieve this goal. Incentives could include glue grants (see Tactic #2 of recommendation P5), workshops, or large multi-organizational research initiatives (either via starting new programs or leveraging existing ones).

#### Tactic #2: Nanoscale to microscale bridging

This stage of the effort would involve bridging from "discrete-to-discrete" models, over finer length scales. This effort could interface with recommendations on nucleation and interface problems in recommendationT5 above, and would likely correspond to a medium term time frame (2–5 years).

#### Tactic #3: Microscale to mesoscale bridging

This stage would involve bridging (via constitutive equations) from "discrete-to-continuous" and/ or "continuous-to-continuous" models, over larger length scales, and would be a medium term endeavor as well.

#### Tactic #4: Integration of results from Tactics #2 and #3

This would involve integrating the bridges developed in Tactics #2 and #3, and would likely not be completed in five years or more from now. Both this tactic and Tactic #3 would also leverage results

from recommendation P6 further below (developing a single, 4D publicly available experimental dataset).

### <u>Recommendation T7</u>: Develop new, verified, and validated methods to inform/derive atomic potentials

This recommendation is centered about "data-derived" interatomic potentials, perhaps involving a blending of bottom-up and top-down strategies which take into account new atomic environments. These potentials will help bridge scales from the DFT regime into larger scale simulations for example involving dislocations (angstroms to nanometers), and bridge timescales from those associated with DFT runs (~picoseconds) to access accelerated dynamics methods in the regime of microseconds or seconds. These efforts could involve collaborations between materials scientists and chemists, physicists, computer scientists, mathematicians, statisticians, and data scientists.

### <u>Tactic #1</u>: Develop best practices, new algorithms, and standardized codes for fitting interatomic potential models and for assessing their transferability

This would include the ability of models to describe new atomic environments; i.e., in a manner in which the potentials could be transferred amongst different atomic environments. Development of unified approaches and broadly applicable algorithms and tools could be a long-term endeavor.

<u>Tactic #2</u>: Approach issues of validation and uncertainty quantification (UQ) in an efficient manner In the medium time frame (3–5 years), as algorithms and tools to produce enhanced new interatomic potentials are under development, it will be important to employ methodologies for handling validation and UQ issues efficiently, in order to make the problem more tractable.

#### Tactic #3: Develop good practices for sharing and checking of potentials

It is imperative that the researchers working in this area (materials scientists, chemists, physicists, computer scientists, mathematicians, statisticians, and data scientists) make strong efforts to share and check potentials across the various research groups and communities that use this data. This could include sharing of data via publication vehicles, large scale repositories supported by government agencies or consortia, and/or large collaborative research projects. Such sharing practices would need to be initiated in the short term, to support development of the new algorithms and potentials.

### <u>Recommendation T8</u>: Develop predictive scaling laws and identify transitions for complex collective phenomena; i.e., emergent phenomena

Development of scaling laws and identification of related transitions (or breakdown points) in "emergent" mesoscale phenomena would provide another important vehicle to support bridging of predictive materials simulations across length and time scales. "Emergent phenomena" refer to higher scale patterning of defects or other aspects of microstructure that arise from many body interactions and can manifest non-intuitive large-scale collective behavior. In other words, these phenomena emerge from interactions at a lower scale and often take the form of power-law relationships between physical quantities. Knowing such relationships allows microstructural simulations of smaller scales to predictively inform what happens at larger—and more relevant—scales. Different scaling laws could apply to emergent phenomena across many different length scales; one example

would be scaling laws and transition points applied to dislocation patterning, in order to bridge from the nanometer to the micron scale range. However, beyond knowing that scaling laws exist, or even the values of the exponents, we require information about the *applicability* of these laws so that smaller scale simulations are truly relevant to the material length- and time-scales of interest. This recommendation would best be addressed by glue grants that allow scientists and engineers to selforganize across different areas of expertise that might include applied mathematics, physics, and theoretical and experimental materials scientists.

#### Tactic #1: Hold workshops

It would be helpful to hold a series of workshops, inviting mathematicians, physicists, and theoretical and experimental materials scientists who have interest in this area. These experts could work together to identify relevant classes of emergent phenomena in materials modeling, and initiate research projects and collaborations that would address development of scaling laws and identification of transition points. For example, some workshops in this area might be organized by the Center for Nonlinear Studies (CNLS) at Los Alamos National Laboratory, which organizes research related to nonlinear and complex systems phenomena. Workshops such as this should be executable in the short term (over the next 3 years).

#### Tactic #2: Validate low-order physical interactions in predictive scaling laws

This would allow for improved scaling laws to permit extrapolation from smaller scale simulations to larger scales. A specific example here would be addressing dislocation-dislocation interactions for the development of dislocation cell structures, including validating new or enhanced scaling laws which link the dislocation-dislocation interactions to the cell structure development. These types of efforts could probably be accomplished in the medium timeframe (3–5 years)

<u>Tactic #3</u>: Develop automated approaches to extract scaling laws from arbitrary (small) simulations The goal here would be the development and implementation of automated methodologies and codes that extract the scaling laws from a variety of existing materials simulations (and their output data). This would likely take a longer time to accomplish (5–10 years), in terms of robust, automated tools being implemented throughout the MSE community.

#### Recommendation T9: Develop methods to automatically update linkage models

"Linkage models" refers to models that link other models and data across length and/or time scales, and here consideration is given not only to such linkage models that may already exist (e.g., see Section IIC.), but very importantly, to models that are yet to be developed as well. Automatic updating could encompass, for instance, flagging models that "fall out" of validation under certain conditions, and the need for them to be adjusted on the fly to bring them back within the proper bounds. This could involve research to incorporate uncertainty quantification and propagation (UQ/ UP) into linkage model development, as well as adaptive methods that deal with multiple protocols (different ways of linking models) or data streams (similar to a workflow model such as iSight<sup>™</sup>). Fault detection and tolerance<sup>r</sup> in the face of evolving data (experimental and/or computational) that

r. Fault tolerance generally refers to the property that enables a system to continue operating properly in the event of the failure of some of its components. A fault-tolerant design enables a system to continue its intended operation, possibly at a reduced level, rather than failing completely, when some part of the system fails (e.g., see www.wikipedia.org)

becomes invalid during simulation runs is also an issue to consider here. Additionally, computer programs within linkage models need intelligent assessment of data passing (e.g., intelligent, efficient APIs), within multiscale frameworks such as CALPHAD, LS-DYNA<sup>TM</sup>, Abaqus<sup>TM</sup>, or others.

Specific initiatives here could benefit from the efforts of a variety of researchers, including those from multidisciplinary design optimization communities (e.g., within aerospace engineering, mechanical engineering, civil engineering, and others), computer science, data science, and materials science and engineering.

#### Tactic #1: Establish various community linkages for specific problems

For example, in the short term, materials scientists could begin working with computer scientists and data scientists on issues such as fault detection and tolerance.

#### Tactic #2: Interface APIs and data infrastructure

This could likely be addressed in the medium timeframe, and is related in the longer term to recommendation P1 below as well.

#### Tactic #3: Consider these methods during new/evolving model development

This could likely be addressed in the medium timeframe. As methods for automatically updating linkage models become more commonplace, the development of new materials models should be planned with such linkages in mind. This will help the community's efforts to build a suite of seamlessly integrated models that facilitate length- and time-scale bridging.

#### Tactic #4: Create robust, adaptive tools that are materials-domain agnostic

It is important to develop linkage tools that are not only adaptive (can update automatically), but that can also be applied over a wide range of materials systems. Development of such robust tools would likely be a long time frame endeavor.

#### Tactic #5: Develop reduced order models for smart sampling across scales

See the first entry of Table 3A above (gaps and limitations) for a brief discussion of reduced order modeling, and also the related Tactic #2 of recommendation P7, below.

#### **Programmatic Recommendations**

#### Recommendation P1: Establish an infrastructure for multiscale materials data

It is important to establish an infrastructure for databases for multiscale materials data; i.e., a group of linked databases for materials data (recognizing that a single database is unrealistic). This infrastructure should include both experimental and modeling data covering the entire range of length scales (from atoms to meters). It could be organized along length scales (e.g., databases for atomistic data, ones for microstructural data, etc.), but could just as well use other organizational schema (e.g., material category). Building such an infrastructure would take a long-term commitment from a range of communities working together, including the existing materials data community, the data science community, federal agencies, policy makers (e.g., journal makers/editors), and other

key stakeholders (such as large companies), and would be a strong supporting component of the Materials Genome Initiative (MGI) "materials innovation infrastructure".<sup>19,20</sup> Although this is a huge endeavor which would encompass many efforts and tactics, some "thought starter" possibilities are provided below.

<u>Tactic #1</u>: *Engage other communities with experience in this area for lessons learned* For example, the biology and astronomy communities have developed similar types of data infrastructure, and before reinventing the wheel, the materials community should study the relevant practices within those other fields.

<u>Tactic #2</u>: *Explore commercial routes for establishing such an infrastructure of federated databases* For example, perhaps reach out to Google to see if they have interest in helping organize materials data in this way, perhaps by providing some tools, services, and/or experience and expertise that could be applied to such an effort.

<u>Tactic #3</u>: *Work with various agencies to facilitate establishment of a database network* For example, work with NIST, DOE, Department of Defense (DoD), National Science Foundation (NSF), and other MGI-related agencies<sup>20</sup> to catalogue any databases they have already established, and whether they would be willing to work together to create such an interwoven network.

### <u>Recommendation P2</u>: Create a network(s) for computational materials science that can help address challenges associated with multiscale modeling and simulation

An example of such a strategy from other disciplines are Mathematics and Physics Institutes (e.g., at the University of Minnesota, UCLA, Berkeley, the Aspen Institute) that address common overarching challenges in the field. Similarly, a computational materials science and engineering "network" or institute could be developed to help address challenges in computational materials science and engineering, including those associated with bridging length and time scales across predictive simulations. In the short term, such a network could help convene workshops, symposia, and/or conferences, to identify specific challenges and recommend solutions, and solution pathways. Such a network could also promote workforce development though curriculum recommendations and development, and develop short courses for postdoctoral researchers, graduate students, or even undergraduates.

#### Tactic #1: Create the network or individual institutes

In order to emulate the success of such networks in fields such as math and physics, the computational materials science community should identify the key priorities of the community and seek out individuals with the right expertise to pursue these interests. Attention should be given to ensure a wide diversity of experts from government, academia, and industry. The ultimate goal of this network would be the development of productive collaborations towards addressing the technical challenges associated with multiscale modeling and simulation.

#### Tactic #2: Convene workshops, symposia, and conferences

Once the network (or individual institutes) for computational materials science are assembled, researchers within these groups should be regularly convened via workshops, symposia, and conferences in order to encourage information exchange and the development of cross-organizational

collaborations. These events should be particularly oriented towards defining pathways for the development of new length- and time-scale bridging strategies and the optimization of existing methods. A key enabling factor in improving the state of the art is bringing the right researchers together to tackle these issues.

#### Tactic #3: Address curriculum recommendations and development

Creating a network (or set of institutes) focused on computational materials science holds promise not only for advancing the state of the art in this area, but also for passing this progress down to upcoming generations of materials scientists, data experts, software engineers, and others. Thus, a focus of such bodies should be the development or modification of undergraduate and graduate school curricula. A particular emphasis of such curricula could include an increased focus on crossdisciplinary work amongst computer science and materials science and engineering majors.

#### Tactic #4: Develop short courses

In addition to making recommendations regarding curricula, the network or set of institutes should also pursue strategies to make their findings known to other computational materials scientists as well as the broader materials science and engineering community. A potential vehicle for this would be the development of short courses that encapsulate the findings of research groups in this area.

### <u>Recommendation P3</u>: Develop a set of mechanisms for increasing the coordination of international multiscale modeling efforts

This recommendation stems from recognition of the strong multiscale modeling efforts taking place both in the US and internationally. In particular, coordinating bodies such as the European Materials Modeling Council (EMMC) and strong modeling projects within a number of European countries speak to the high priority of the development of multiscale modeling capabilities in those regions, while other significant efforts worldwide are being led by researchers from China, Japan, Canada, and more. Thus, in order to further stimulate success in this discipline, mechanisms are needed to increase international collaborations and coordination of multiscale modeling efforts.

#### Tactic #1: Convene international expert panels to develop roadmaps and encourage networking

Short workshops and brainstorming sessions amongst experts from multiple nations should be convened to develop roadmaps for collaborative activities and to provide venues for international networking within the multiscale modeling community. Strong facilitation of these meetings and a commitment to content capture and dissemination will help ensure their value to the community. Such meetings could be held independently or collocated with existing conferences in related topical areas.

#### Tactic #2: Convene multiscale modeling researchers virtually

In addition to in-person meetings and brainstorming sessions, virtual forums and web resources could be used to greater effect for information sharing and collaboration in the multiscale modeling arena. Potential venues for such interactions include online forums such as the Integrated Computational Materials Engineering expert group (ICMEg) discussion forum<sup>s</sup>. Smaller scale virtual meetings or webinars on focused topics could also serve as strong venues for encouraging international collaboration on niche topics.

s. www.icmeg.euproject.info/forum/integration-platforms/32-existing-platforms.html

#### Tactic #3: Create research funding opportunities jointly between multiple nations

A key component of bringing to bear the research capabilities of universities and other non-profit research institutions on a problem is the availability of funding support. In light of this, a strong mechanism for encouraging researchers from multiple world regions to leverage each other's capabilities in multiscale modeling would be for countries to create joint funding opportunities in this area, stipulating a strong component of international collaboration in proposed research.

### <u>Tactic #4</u>: Define a set of Foundational Engineering Problems (to be pursued by the global modeling and simulation community)

Defining and publishing a set of Foundational Engineering Problems (FEPs) in the area of multiscale modeling could be an important enabler to galvanize multinational collaboration. Focusing on challenges which entail significant intellectual and computational resource allocation would help necessitate coordination of many researchers across multiple regions, while ensuring that success, if achieved, would have significant value to the field as a whole. These problems should be identified by a combination of researchers from various industries to guarantee relevance to real life engineering scenarios.

### <u>Recommendation P4</u>: Incentivize the community to develop Application Programing Interfaces (APIs) and standards for connecting different computational tools across length scales

This recommendation applies more to *implementation* via computational tools that pass data back and forth between different models, as opposed to linking at the more fundamental model or algorithm stage. Efforts here would likely involve materials scientists and engineers collaborating with software engineers, computer scientists, and others within the scientific computing community (e.g., specifically for improving the efficiency of APIs). Some possible approaches to act on this recommendation include:

### <u>Tactic #1</u>: Convene groups of experts to identify state-of-the-art API technologies and available computational materials codes

This could involve both commercial and open access computational materials codes. Industrial users would be of particular value in helping set standards and requirements for APIs. This tactic could include workshops that specifically and clearly identify and formalize input/output needs at different length scales. Collaborations amongst groups who do modeling and simulation at different length and time scales should be fostered, to allow for development of APIs of the highest impact for the materials modeling community. Convening of such expert groups toward this goal should be undertaken in the short term.

### Tactic #2: Incentivize API development through SBIRs (industry) and specific research programs (academia and national laboratories)

The key here is to support and build specific research programs focused on API development. Small Business Innovation Research (SBIR) programs with the goal to support API development could stimulate industrial groups in this regard, while other types of research programs targeted at API development would need to be supported at universities and in national laboratories. The focus of these specific, individual research programs would be on APIs related to multi-scale applications,

perhaps across regimes including: (1) quantum-to-atomistic, (2) atomistic-to-microstructure scale, and (3) microstructure-to-continuum scale. Obtaining support for, setting up, and executing such research programs would likely be accomplished in the medium time frame (3-5 years) at best.

Tactic #3: Develop data translators and information passing protocols (for inputs-outputs)

One of the major difficulties arising when attempting to integrate heterogeneous materials simulation tools is the fact that the data corresponding to inputs and outputs of the codes—which can in turn constitute inputs to other codes—are represented in often incompatible formats. In some cases, commercial code developers choose proprietary and closed data encapsulation formats. Even in the case of open source codes, however, data format incompatibility is the norm rather than the exception.

Tactic #3 addresses this issue by calling for the development, through collaborative efforts, of automatic data translators and/or information passing protocols that can be used to convert some of the inputs and outputs of simulation tools into compatible formats. This action item could potentially be carried out within existing research programs, or through community-based collaborative efforts and thus could be actionable in the short term.

One of the major issues associated with combining computational tools is the lack of standards for representing materials data. Metadata standards for materials are needed so that software tools can easily identify and pass data from one tool to another. Ideally, the same types of materials properties would be represented in similar ways by different computational tools. Although there have been some efforts towards this goal, there is currently no major initiative tackling this problem.

#### Tactic #4: Establish standards for materials data representation

One of the major issues associated with combining computational tools is the lack of standards for representing materials data. Metadata standards for materials are needed so that software tools can easily identify and pass data from one tool to another. Ideally, the same types of materials properties would be represented in similar ways by different computational tools. Although there have been some efforts towards this goal, there is currently no major initiative tackling this problem. Since significant buy-in from the community is necessary—in the United States and abroad, across universities, national laboratories and industry—this is considered a medium- to long-term endeavor. Considerable work has recently taken place at the macro-scale to couple multi-physics models, resulting in the development of multi-physics interfaces<sup>t</sup> and perhaps there are ideas from this community that can be applied to materials science and engineering (MSE) to incentivize the adoption of a common standard for data translation.

t. e.g., see www.mpcci.de/mpcci-software.html

### <u>Tactic #5</u>: Establish connections between materials science and computer science faculty and students

Materials science and computer science faculty should consider working together as joint Ph.D. (or masters) student thesis advisors, on specific research projects that have components centered about developing API implementations and standards aimed at connecting computational tools (related to materials modeling) across length and time scales. Such cross pollination is commonly done in other disciplines (e.g., engineering and public policy, medical research and materials science and engineering, etc.), and would be of great value here. There is no reason why such joint research projects could not be undertaken in the short term (3 years or less). Additional interactions could entail recruitment of undergraduate computer science majors to work in research groups within materials science and engineering departments, including possible summer internship programs for undergraduate students.

### <u>Recommendation P5</u>: Support open data mandates for authors to publish data in appropriate repositories as part of journal submission requirements

Access to many forms of materials data (both experimental and modeling data) by the broadest possible user base is pivotal for the community to make great strides in bridging materials models across length and time scales. This would apply to data across all length scales. In the context of journal publications, "data" can be taken to mean various forms of information needed to reproduce the published results. Examples of such supplementary data might include: (1) DFT models - input parameters, and all outputs (e.g., not just convex hull plots); (2) diffusion studies—raw data such as intensity vs. distance profiles, composition profiles, etc.; (3) CALPHAD assessments—evaluated data files such as the input "POP" files, not just phase diagrams or free energies of formation for example; (4) microstructure data—rather than just the final microstructure representations, this might include data such as atom probe "POS" files, or the raw data from a serial sectioning experiment. Additionally, it is best for such data not to be limited to subscribers only, but instead it should be openly accessible to the entire community.<sup>42</sup>

Fully addressing this recommendation would require cooperation amongst materials scientists and engineers, data informatics experts, computer scientists, statisticians, and journal editors and publishers.

#### Tactic #1: Develop solutions for large data transfer and storage

As characterization techniques advance, large amounts of data are generated (e.g., one scattering experiment at the Advance Photon Source may generate 5 terabytes of data) that need to be shared with a variety of researchers. A data infrastructure that supports access and transfer of large data files is essential. Cloud-based data storage is one potential solution<sup>u</sup>.

#### Tactic #2: Develop metadata descriptions

Metadata descriptions are needed to tag data so that it can easily be identify by search tools. Metadata descriptions will not only enable data to be identified and used, but is also essential for the development of data mining and analysis tools.

u. For example, see globus.org/

Data provenance refers to the process of tracing and recording the origins of data and its movement between databases,<sup>86</sup> as well as across models or amongst different researchers. Since data is a critical component of all materials modeling and bridging across materials models, the tracking of data provenance is critical to a number of issues including the accuracy/validity of the data, uncertainty quantification and error propagation, and model validation.

#### Tactic #4: Develop new incentives for data sharing

New incentives for data sharing could involve strategies such as exploring e-collaboration, game theory research into the ways people collaborate, or creative ways of making data sharing one of the metrics considered during the tenure evaluations of faculty members.

# <u>Recommendation P6</u>: Convene the community to identify a large (statistically relevant), single, 4D publicly available experimental dataset to serve as the focal point of a community-wide case study in multiscale modeling approaches

The MSE community should be the primary group addressing this recommendation, perhaps with some interactions with the statistics community. Development of the dataset(s) would not only involve experimentalists, but would also require guidance from modelers to help identify the types of 4D (i.e., 3D plus time) data that would have the most significant impact on subsequent multi-scale modeling efforts. This dataset recommendation would apply from the lowest length scale that can be resolved with the techniques employed (perhaps nanometers) up to millimeters (or even centimeters). Addressing this recommendation would also provide leverage for recommendations P4 and T6, and have some relevance to recommendation T1 as well.

#### Tactic #1: Create a robust, experimentally measured 4D dataset

This could involve a single well-supported research group effort, or multiple research groups working together on a common problem. Creation of this robust dataset would create a strong resource for the MSE community to support model validation and to serve as input for various modeling and simulation efforts. Development of this dataset is estimated to be at least a medium term endeavor (3–5 years). Due to the 3D and temporal elements, this could involve high-throughput, high-resolution synchrotron techniques, perhaps supplemented by in-situ microscopy techniques, as well as destructive serial sectioning techniques to serve as the final experiments on the specimen(s) used for the in-situ (and/or ex-situ) non-destructive work. Any complementary experiments should be performed on the same specimen(s) if at all possible (or at least the same material and processing conditions). In order to fully leverage with related modeling efforts and present valuable challenge problems for the computational use cases, it is recommended that such a dataset(s) be developed for a materials system (or alloy) containing at least four or five elemental components.

#### Tactic #2: Quantify uncertainty and verify self-consistency of the 4D dataset

It is estimated that this activity could be performed in the medium time frame. This effort is related to the fact that it is not sufficient to just develop a robust 4D dataset, but verifying its self-consistency is critical. One method to accomplish this would be via a combination of multiple, repeated experiments using a single technique, as well via cross checking with multiple experimental techniques. Additionally, in order to use this experimental data set as input for multiple models and

simulations, it will be important to quantify the level of uncertainty associated with the data (see also recommendation T1).

#### Tactic #3: Distribute the data to modelers

It is imperative that this data be distributed to a wide range of modelers (over as many modeling length and time scales as relevant) in order to make the broadest impact possible. Once the dataset is completed, this distribution should be feasible in the short term (less than 3 years after the data is developed).

#### Tactic #4: Develop protocols for exchange of the data

This would be one of the final steps in this recommendation and would support many computational teams from various groups reproducing the data and using it for direct, quantitative validation of models. Development of such protocols should be able to be accomplished in the short term.

#### Tactic #5: Continually re-convene the community to evaluate and use these results

This is a long-term proposition and involves a continual re-evaluation and use of the robust 4D data developed, and continual assessment of its implications on various modeling efforts.

### <u>Recommendation P7</u>: Develop a suite of physically based analysis tools (including standard protocols for performing spatial correlations and statistics)

A robust suite of physically based<sup>v</sup> analysis tools that are available to the materials discovery and development communities can facilitate materials modeling across length and time scales, irrespective of the materials type or application, or the specifics of the individual models and codes being employed. These analysis tools should also be augmented with standard protocols for performing spatial correlations on microstructures and other features at various length scales (e.g., atoms at nanoscales, phase sizes and distributions at the mesoscale), as well as various types of statistical analysis tools applied to microstructure attributes and/or property measurements. These tools could apply to bridging efforts across the entire length scale regime (angstroms to meters). This recommendation would best be addressed by scientists and engineers across a spectrum of expertise areas including materials science and engineering, signal processing, information and data sciences (computer science, informatics), image analysis, uncertainty quantification, multidisciplinary design optimization, and mechanics of materials. This recommendation also dovetails with recommendations T6 and P6.

#### Tactic #1: Data analysis tools for high-throughput methods

An important set of tools within this suite would include those that provide for efficient analysis of large amounts of data obtained from high throughput methods (e.g., see recommendation T5, Tactic #1). Development of some of these analysis tools would likely encompass a short- to medium-term effort.

v. "Physically based" in this context refers to tools that are based on underlying physics, or physical principles and/or behavior, as opposed to completely generalized tools for scientific analysis.

#### Tactic #2: Community analysis tools based on reduced-order methods<sup>w</sup>

Development of initial reduced-order analysis tools could likely be accomplished in the medium time frame (3–5 years); whereas increasingly physically-rooted reduced-order methods might take longer to develop and implement. It is important to ultimately develop reduced order models and tools that allow for intelligent sampling across a wide range of length and time scales.

w. Reduced-order approaches refer to methodologies that reduce the number of degrees of freedom for the model description in order to make the problem or analysis more tractable or to move, for instance, from a dynamic to thermodynamic description. Reduced-order models of various sorts are commonly introduced to bridge across mesoscales of material structure.



# V. Closing Remarks and Call to Action

The value of materials modeling from the atomic scale through the mesoscale to the scale of applications has been demonstrated in the last decade by the emergence of Integrated Computational Materials Engineering (ICME) and the Materials Genome Initiative (MGI), offering great promise for providing large reductions in the time and cost of developing new and improved advanced materials and manufacturing process innovations. A crucial element needed for implementing predictive materials models and simulations into materials design and development is their integration by bridging across length and time scales. Despite a number of publications that have discussed the value of multiscale materials modeling, there remain many gaps and limitations (see section III) in fundamental models, implementation methodologies, and computational codes that provide integration and linkage of materials modeling and simulation across length and time scales. Addressing those gaps and limitations was the subject of this study.

One overarching finding of this study is that in addition to modelers and experimentalists within the materials science and engineering (MSE) community, experts from other communities must also contribute to addressing many of the limitations and recommendations presented in this report. As discussed throughout Section IV, beyond researchers in the MSE community, there is a need for engaging others in this discussion including experts in the fields of mechanics of materials, statistics, applied mathematics, signal processing, computer science, image analysis, data sciences and informatics, software engineering, physics, chemistry, mechanical engineering, chemical engineering, manufacturing and processing, and multidisciplinary design optimization.

This report addresses important issues associated with the integration and linkage of materials models and simulations across length and time scales, and makes a number of specific recommendations toward that end (in section IV). Readers can use this information to assist in activities such as the development of fundamental linkage models, implementation strategies, quantitative computational codes, and creative new ways for engaging and convening the community to address the challenges associated with bridging materials models across length and time scales. It is emphasized that the specific recommendations and tactics presented in the report (Section IV) should in no way be viewed as all-inclusive, and researchers, leaders, and policy makers who read this report are also challenged to use this information to stimulate the development and execution of additional new tactics for addressing the gaps and limitations, and accomplishing the recommendations identified in this study.

It is our desire that the readers of this report will act promptly on its recommendations. There is much work to be done, and there is great potential for making both important short-term progress, as well as great strides in the longer term in the effort to bridge materials models across length and time scales and produce the predictive models that the community so desperately needs.

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# VII. Appendix

Appendix: Software codes discussed in the report including brief descriptions and hyperlinks. Where quoted, descriptions are excerpted from the corresponding hyperlinks.

Software Name	Description	Open Source or Commercial (O/C)
µMatIC	"The µMatIC code is a combination of a finite difference solute diffusion solver with a volume of fluid style scalar implemented to track the solid-liquid-gas interface." https://workspace.imperial.ac.uk/advancedalloys/ public/software/uMatIC_usermanual_V2.pdf	0
Abaqus	The Abaqus Unified FEA (finite element analysis) product suite performs "virtual tests with realistic simulation which helps reduce product development time and costs, while improving reliability." <u>http://www.3ds.com/products-services/</u> <u>simulia/portfolio/abaqus/overview/</u>	С

ABINIT	ABINIT allows calculation of the total energy, charge density and electronic structures of molecules and periodic solids within "Density Functional Theory (DFT), using pseudopotentials and a planewave or wavelet basis." ABINIT also allows geometry optimization, molecular dynamics simulations, and more using the DFT forces and stresses. http://www.abinit.org/	0
Accelrys Materials Studio	The Materials Studio modeling environment supports predictions and investigations of materials' structure-property relationships. The modeling environment includes solution methods for quantum, atomistic, mesoscale, and statistical methods for evaluating various particle sizes and time scales. Crystal structure and growth evaluations are also supported. http://accelrys.com/products/materials-studio/	С
ALE3D	"ALE3D is a 2D and 3D multi-physics numerical simulation software tool using arbitrary Lagrangian-Eulerian (ALE) techniques. The code is written to address both two-dimensional (2D) and three-dimensional (3D) problems using a hybrid finite element and finite volume formulation to model fluid and elastic-plastic response on an unstructured grid." https://wci.llnl.gov/simulation/computer-codes/ale3d	0
Ansys	The Ansys product suite employs finite element analysis software products to solve a wide variety of engineering and design problems. http://www.ansys.com/	С
ATAT	The Alloy-Theoretic Automated Toolkit (ATAT) includes tools for: cluster expansions from first-principles (MAPS), Monte Carlo simulation of lattice models in order to compute thermodynamic starting from a cluster expansion, extending the above tools to reciprocal-space cluster expansions, and interfacing the above tools with first-principles codes (such as VASP). http://www.brown.edu/Departments/Engineering/ Labs/avdw/atat/manual.pdf	Ο
ATK	ATK (Atomistix ToolKit) is an atomistic simulation software supporting functionalities such as an atomic 3D builder platform and a variety of analysis and calculation methods. http://quantumwise.com/	С
Autoform	AutoForm software supports simulation and planning of manufacturing processes for the die-making and sheet metal forming industries. Supported functions include stamping, die design, thermodynamics solvers, and process planning. http://www.autoform.com/en/	С
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CASINO	"CASINO is a computer program system for performing quantum Monte Carlo (QMC) electronic structure calculations that is capable of calculating accurate solutions to the Schrödinger equation of quantum mechanics for realistic systems built from atoms." http://vallico.net/casinoqmc/	O (for academics/ non-profits)
CD-adapco	CD-adapco software packages support a wide range of computational fluid dynamics (CFD) and finite element analysis (FEA) problem sets. http://www.cd-adapco.com/	С
CLUPAN	CLUPAN uses the cluster expansion method to calculate atomic configuration effects, ground state structures, thermodynamic quantities, equilibrium diagrams, and disordering by temperature. http://ma.cms-initiative.jp/en/application-list/clupan/clupan	0
Comsol Multiphysics	"COMSOL Multiphysics <sup>®</sup> is a general-purpose software platform, based on advanced numerical methods, for modeling and simulating physics-based problems." http://www.comsol.com/comsol-multiphysics	С
CPMD	"The CPMD code is a parallelized plane wave / pseudopotential implementation of Density Functional Theory, particularly designed for ab-initio molecular dynamics." http://cpmd.org/	0
CRYSTAL	The CRYSTAL program facilitates the study of crystalline materials by computing the electronic structure of systems within various approximations including Hartree Fock and density functional theory. http://www.crystal.unito.it/index.php	С
DANTE	"DANTE is a coupled thermal, carbon diffusion, solid mechanics finite element based program for simulating the heat treatment of steel parts." http://www.dante-solutions.com /	С

DEFORM	DEFORM simulates and allows analysis of machining, mechanical joining processes, metal forming, and heat treatment in order to optimize processes in terms of cost and performance. http://www.deform.com/	С
DICTRA	"Software for accurate simulation of diffusion controlled reactions in multi-component alloy systems, which is based on numerical solution of the multi-component diffusion equations." http://www.thermocalc.com/products-services/software/dictra/	С
DIGIMAT	A multi-scale material and structure modeling platform for composite materials. Digimat allows micro- and macro-scale analyses of composites, predicting mechanical, thermal and electrical properties and performance for use in downstream finite element analysis. http://www.mscsoftware.com/product/digimat	С
DREAM3D	DREAM3D allows reconstruction and analysis of experimental or simulated 3D microstructures. It also allows creation of microstructures using data from real world materials or through user generated statistics. http://dream3d.bluequartz.net/	0
DYNAFLOW	Dynaflow software platforms allow simulations in "the fields of gas liquid interface dynamics, bubble dynamics, cavitation, fluid structure interactions and erosion dynamics." <u>http://www.dynaflow-inc.com/</u>	С
EMC2	"EMC2 is a mixed R/C program designed to carry out multi-scale spatial modeling of Poisson events data." http://hea-www.harvard.edu/AstroStat/EMC2/	0
FactSage	FactSage© is an integrated database computing system in chemical thermodynamics.	С
GPAW	"GPAW is an efficient program package for electronic structure calculations. It is based on the density-functional theory implemented within the projector augmented wave (PAW) method using uniform real-space grids." https://research.csc.fi/-/gpaw	0

GULP	GULP performs materials simulations focusing on analytical solutions via lattice dynamics using "boundary conditions of 0-D (molecules and clusters), 1-D (polymers), 2-D (surfaces, slabs and grain boundaries), or 3-D (periodic solids)." http://nanochemistry.curtin.edu.au/gulp/	0
HT Tools	"HT-Tools is a simulation software that models and optimizes carburizing processes before implementation, plotting the carbon diffusion and hardness profiles." http://www.group-upc.com/mf/eng_mf/Heat/HT_Tools.htm	С
iSight and the SIMULIA Execution Engine	"Isight and the SIMULIA Execution Engine (formerly Fiper) are used to combine multiple cross-disciplinary models and applications together in a simulation process flow, automate their execution across distributed compute resources, explore the resulting design space, and identify the optimal design parameters subject to required constraints." <u>http://www.3ds.com/products-services/simulia/</u> <u>products/isight-simulia-execution-engine/</u>	С
LAMMPS	"LAMMPS is a classical molecular dynamics code, and an acronym for Large-scale Atomic/Molecular Massively Parallel Simulator. LAMMPS has potentials for solid-state materials (metals, semiconductors) and soft matter (biomolecules, polymers) and coarse-grained or mesoscopic systems." http://lammps.sandia.gov/	0
LS DYNA	LS-DYNA is a general-purpose finite element program enabling solutions for coupled multi-physics problems. Examples of specific applications include: nonlinear dynamics, quasi-static simulations, failure analysis, and crack propagation. http://ls-dyna.com/	С
Magma	Magma software products support casting process simulations to help optimize foundry manufacturing and operations. http://www.magmasoft.com/en/	С
Marmot	Part of the MOOSE simulation framework, MARMOT models microscopic changes in nuclear fuel during irradiation. http://www.inl.gov/research/moose-applications/	0

MatCalc	"MatCalc is software for computer simulation of phase transformations in metallic systems. "The thermodynamic foundation of MatCalc is the CALPHAD method and (unencrypted) CALPHAD-type databases. The kinetic modules of MatCalc are developed within the framework of solid-state phase transformations, with particular focus on computational efficiency and applicability to multi-component systems." <u>http://matcalc.tuwien.ac.at/</u>	С
MatForge	"As part of the NSF NSDL, MatDL Pathway provides a branded, trusted, non-commercial, and neutral site supporting open source, collaborative, materials code development." <u>http://matforge.org</u>	ο
Micress	MICRESS® - the MICRostructure Evolution Simulation Software - is a software enabling the calculation of microstructure formation in time and space during phase transformations, especially in metallurgical systems. <u>http://web.access.rwth-aachen.de/MICRESS/</u>	С
ModelCenter	ModelCenter® is a graphical environment for automation, integration, and design optimization that allows users to "quickly create an engineering process and then explore the design space to find the best design." http://www.phoenix-int.com/software/phx-modelcenter.php	с
Modelica	"Modelica® is a non-proprietary, object-oriented, equation based language to conveniently model complex physical systems containing, e.g., mechanical, electrical, electronic, hydraulic, thermal, control, electric power or process-oriented subcomponents." <u>https://www.modelica.org/</u>	0
Moldflow	"Simulation Moldflow® software provides tools for injection mold design, plastic part design, and the injection molding process." http://www.autodesk.com/products/simulation-moldflow/overview	С
MOOSE	"The Multiphysics Object-Oriented Simulation Environment (MOOSE) is a finite-element, multiphysics framework primarily developed by Idaho National Laboratory." http://mooseframework.org/	0

NWCHEM	NWChem provides "computational chemistry tools that are scalable both in their ability to treat large scientific computational chemistry problems efficiently, and in their use of available parallel computing resources from high-performance parallel supercomputers to conventional workstation clusters." http://www.nwchem-sw.org/index.php/Main_Page	0
NX NASTRAN	NX Nastran is a finite element modeling software optimized for structural and component analysis applications. <u>http://www.plm.automation.siemens.com/</u> <u>en_us/products/nx/for-simulation/</u>	с
OOF	OOF software supports finite element analysis of microstructures by "helping materials scientists calculate macroscopic properties from images of real or simulated microstructures." http://www.ctcms.nist.gov/oof/	0
Open CALPHAD	"OpenCalphad is an informal international collaboration of scientists and researchers interested in the development of high quality software and databases for thermodynamic calculations for all kinds of applications." http://www.opencalphad.com/	0
OpenPhase	OpenPhase, based on the multiphase field model, performes "phase field simulations of complex scientific problems involving microstructure formation in systems undergoing first order phase transformation." <u>http://www.openphase.de/</u>	0
OpenSees	"OpenSees [is] a software framework for developing applications to simulate the performance of structural and geotechnical systems subjected to earthquakes." http://opensees.berkeley.edu/	0

PAMCRASH	Within the ESI Virtual Performance Solution, PAM-CRASH is dedicated to crash test simulations, and allows the impact of various manufacturing effects on performance to be taken into account. The Virtual Performance Solution method supports multi-scale modeling by isolating local areas to be analyzed with a refined mesh and incorporating this information smoothly in the overall, higher scale simulation. <u>https://www.esi-group.com/software-services/virtual- performance/virtual-performance-solution</u>	С
Pandat	"Pandat software is an integrated computational environment for phase diagram calculation and materials property simulation of multi-component systems based on CALPHAD (CALculation of PHAse Diagram) approach." <u>http://www.computherm.com/index.</u> <u>php?route=product/category&amp;path=33</u>	С
PanPrecipitation	PanPrecipitation software supports "simulation of precipitation kinetics during heat treatment processes." http://www.computherm.com/index.php?route=common/home	С
ParaDIS	"ParaDiS is a code for doing Dislocation Dynamics simulations and was specifically written to perform well on massively parallel computers." http://micro.stanford.edu/wiki/Overview_of_ParaDiS_2.2	0
FiPy	"FiPy is an object oriented, partial differential equation (PDE) solver, written in Python, based on a standard finite volume (FV) approach." <u>http://www.ctcms.nist.gov/fipy/index.html</u>	0
PHONOPY	"Phonopy is an open source package of phonon calculations based on the supercell approach." Phonopy "calculates crystal phonon properties from input information calculated by external codes, e.g., first-principles calculation code." http://phonopy.sourceforge.net/	0
Potfit	"Potfit is a free implementation of the force-matching algorithm to generate effective potentials from ab-initio reference data." http://potfit.sourceforge.net/wiki/doku.php	0

PrecipiCalc	PrecipiCalc is a software for "calculating the 3D multiparticle diffusive precipitation kinetics of multiple phases." http://www.questek.com/filebase/src/Articles/PpCTechSheet2013.pdf	С
ProCAST	ProCAST is a finite element software for casting process simulation. <u>http://www.esi-group.com/software-services/</u> <u>virtual-manufacturing/casting</u>	С
QMCpack	"QMCPACK is an open-source production level many-body ab initio Quantum Monte Carlo code for computing the electronic structure of atoms, molecules, and solids." http://qmcpack.org/	0
Quantum Espresso	"Quantum Espresso is an integrated suite of Open-Source computer codes for electronic-structure calculations and materials modeling at the nanoscale. It is based on density- functional theory, plane waves, and pseudopotentials." http://www.guantum-espresso.org/	0
QWalk	"QWalk is a program developed to perform high accuracy quantum Monte Carlo calculations of electronic structure in molecules and solids. It is specifically designed as a research vehicle for new algorithms and method developments, as well as being able to scale up to large system sizes." https://code.google.com/p/qwalk/	0
SAP2000	SAP 2000 is a finite element software that features a 3D object based graphical modeling environment and a wide variety of analysis and design tools optimized for use by design engineers. http://www.csiamerica.com/products/sap2000	С
SOLIDCast	The SOLIDCast software suite simulates multiple casting types accounting for "variables in sand, investment, and permanent mold castings" and including thermal and volumetric changes during cooling. http://www.finitesolutions.com/Products/SOLIDCast.html	С
SPPARKS	"SPPARKS (Stochastic Parallel PARticle Kinetic Simulator) is a parallel Monte Carlo code for on-lattice and off-lattice models that includes algorithms for kinetic Monte Carlo (KMC), rejection kinetic Monte Carlo (rKMC), and Metropolis Monte Carlo (MMC)." spparks.sandia.gov	0

STAAD.Pro	STAAD.Pro is a finite element software optimized for structural engineering applications. http://www.bentley.com/en-US/Products/STAAD.Pro/	С
Strand7	Strand7 is a full-featured finite element analysis software.	С
SUTCAST	SUTCAST allows prediction of the microstructures of cast metal components and incorporation of this information in macro-microscopic modeling of solidification. http://www.sutcast.com/simulation-software/solutions/ solidification-simulation/microstructure.aspx	С
SwiftComp Micromechanics	SwiftComp Micromechanics (formerly VAMUCH) utilizes a "finite element-based, general-purpose micromechanics code to perform homogenization of heterogeneous materials based on the variational asymptotic method. It can be used to calculate the effective fully-coupled, multiphysical material properties, including thermal, elastic, electric, and magnetic for arbitrary heterogeneous materials with arbitrary microstructure providing a unit cell (UC), or a representative volume element (RVE), can be identified." <u>http://analyswift.com/products/swiftcomp-vamuch- micromechanics-modeling-of-heterogeneous-materials/</u>	С
SysWELD	SysWELD is a software for heat treatment and welding that allows simulation of various welding methods including MIG/MAG, laser, resistance spot welding, etc. http://www.tc-liv.eu/index.php?option=com_conten t&view=article&id=55&Itemid=59&Iang=en	С
TC-PRISMA	"TC-PRISMA is a software package which treats concurrent nucleation, growth/dissolution and coarsening under arbitrary heat treatment conditions in multi-component and multi-phase systems using Langer-Schwartz theory and the Kampmann-Wagner numerical approach." http://www.thermocalc.com/products-services/software/tc-prisma/	С
Thermo-Calc	Software based on the CALPHAD (CALculation of PHase Diagrams) method that performs thermodynamics calculations and includes access to thermodynamic databases for a wide range of materials. http://www.thermocalc.com/start/	С

Towhee	Towhee is a Monte Carlo molecular simulation code which allows the prediction of fluid, solid, and porous phase equilibria under a variety of force fields. Towhee uses atom- based force fields the Gibbs ensemble with an emphasis on algorithms addressing molecule conformation sampling. <u>http://towhee.sourceforge.net/</u>	0
UNCLE	UNiversal CLuster Expansion (UNCLE) "extends standard cluster expansion formalism to the more complicated cases of ternary compounds, as well as surfaces, including adsorption and inequivalent sites." http://iopscience.iop.org/0965-0393/17/5/055003	0
VASP	The Vienna Ab initio Simulation Package (VASP) performs atomic scale modeling via density functional theory (DFT), the Hartree-Fock (HF) approximation, or Greens's functions methods.	С
WIEN2k	WIEN2k performs electronic structure calculations of solids using the "full-potential (linearized) augmented plane-wave ((L)APW) + local orbitals (lo) method" of density functional theory (DFT). http://www.wien2k.at/	С
Zebulon	Zébulon is a non-linear finite element solver software. The code specializes in highly non-linear materials models and also includes thermal and diffusion problems and coupling of these models. http://www.zset-software.com/products/zebulon/	С



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