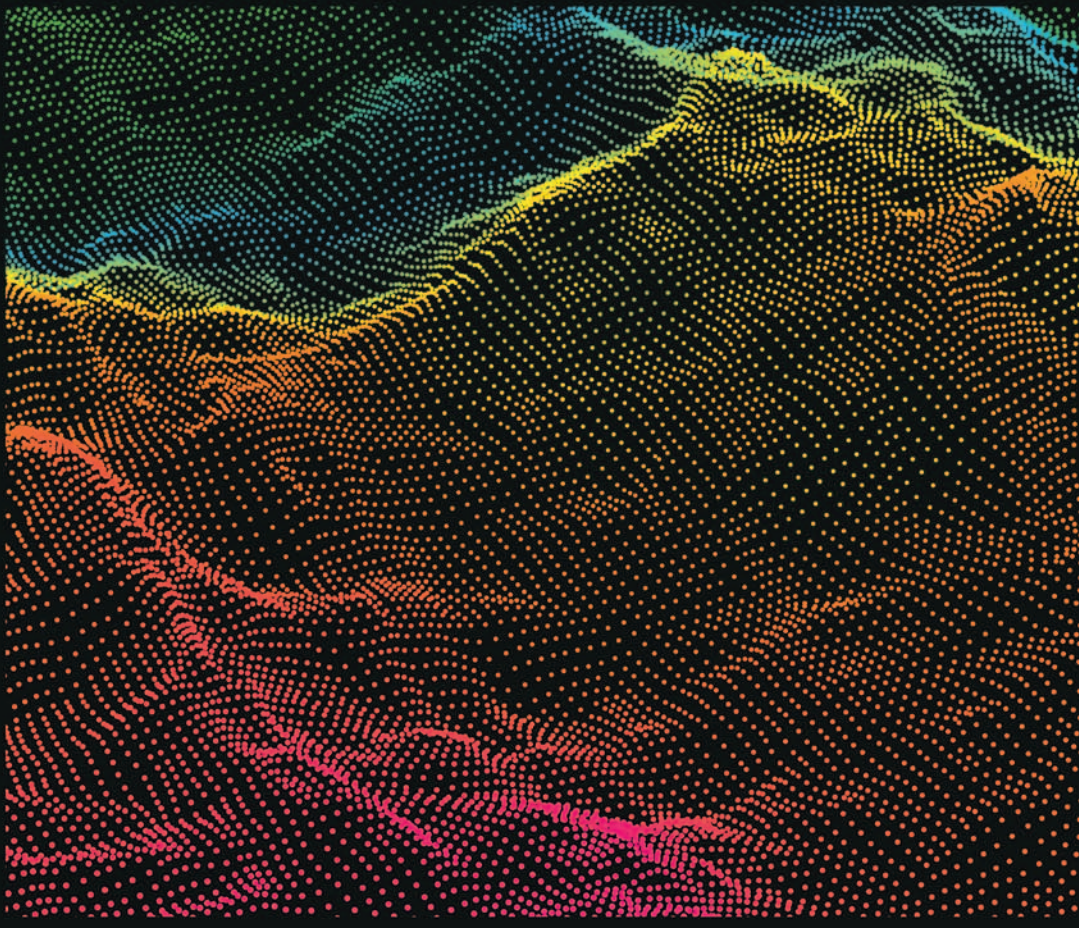
ELSEVIER SERIES IN **MECHANICS OF ADVANCED MATERIALS**

UNCERTAINTY QUANTIFICATION IN MULTISCALE MATERIALS MODELING



Edited by
YAN WANG
DAVID L. MCDOWELL

ELSEVIER

Uncertainty Quantification in Multiscale Materials Modeling

Mechanics of Advanced Materials Series

The Mechanics of Advanced Materials book series focuses on materials- and mechanics-related issues around the behavior of advanced materials, including the mechanical characterization, mathematical modeling, and numerical simulations of material response to mechanical loads, various environmental factors (temperature changes, electromagnetic fields, etc.), as well as novel applications of advanced materials and structures.

Volumes in the series cover advanced materials topics and numerical analysis of their behavior, bringing together knowledge of material behavior and the tools of mechanics that can be used to better understand, and predict materials behavior. It presents new trends in experimental, theoretical, and numerical results concerning advanced materials and provides regular reviews to aid readers in identifying the main trends in research in order to facilitate the adoption of these new and advanced materials in a broad range of applications.

Series editor-in-chief: Vadim V. Silberschmidt

Vadim V. Silberschmidt is Chair of Mechanics of Materials and Head of the Mechanics of Advanced Materials Research Group, Loughborough University, United Kingdom. He was appointed to the Chair of Mechanics of Materials at the Wolfson School of Mechanical and Manufacturing Engineering at Loughborough University, United Kingdom in 2000. Prior to this, he was a Senior Researcher at the Institute A for Mechanics at Technische Universität München in Germany. Educated in the USSR, he worked at the Institute of Continuous Media Mechanics and Institute for Geosciences [both—the USSR (later—Russian) Academy of Sciences]. In 1993–94, he worked as a visiting researcher, Fellow of the Alexander-von-Humboldt Foundation at Institute for Structure Mechanics DLR (German Aerospace Association), Braunschweig, Germany. In 2011–14, he was Associate Dean (Research). He is a Charted Engineer, Fellow of the Institution of Mechanical Engineers and Institute of Physics, where he also chaired Applied Mechanics Group in 2008–11. He serves as Editor-in-Chief (EiC) of the Elsevier book series on *Mechanics of Advanced Materials*. He is also EiC, associate editor, and/or serves on the board of a number of renowned journals. He has coauthored four research monographs and over 550 peer-reviewed scientific papers on mechanics and micromechanics of deformation, damage, and fracture in advanced materials under various conditions.

Series editor: Thomas Böhlke

Thomas Böhlke is Professor and Chair of Continuum Mechanics at the Karlsruhe Institute of Technology (KIT), Germany. He previously held professorial positions at the University of Kassel and at the Otto-von-Guericke University, Magdeburg, Germany. His research interests include FE-based multiscale methods, homogenization of elastic, brittle-elastic, and visco-plastic material properties, mathematical description of microstructures, and localization and failure mechanisms. He has authored over 130 peer-reviewed papers and has authored or coauthored two monographs.

Series editor: David L. McDowell

David L. McDowell is Regents' Professor and Carter N. Paden, Jr. Distinguished Chair in Metals Processing at Georgia Tech University, United States. He joined Georgia Tech in 1983 and holds a dual appointment in the GWW School of Mechanical Engineering and the School of Materials Science and Engineering. He served as the Director of the Mechanical Properties Research Laboratory from 1992 to 2012. In 2012 he was named Founding Director of the Institute for Materials (IMat), one of Georgia Tech's Interdisciplinary Research Institutes charged with fostering an innovation ecosystem for research and education. He has served as Executive Director of IMat since 2013. His research focuses on nonlinear constitutive models for engineering materials, including cellular metallic materials, nonlinear and time-dependent fracture mechanics, finite strain inelasticity and defect field mechanics, distributed damage evolution, constitutive relations, and microstructure-sensitive computational approaches to deformation and damage of heterogeneous alloys, combined computational and experimental strategies for modeling high cycle fatigue in advanced engineering alloys, atomistic simulations of dislocation nucleation and mediation at grain boundaries, multiscale computational mechanics of materials ranging from atomistics to continuum, and system-based computational materials design. A Fellow of SES, ASM International, ASME, and AAM, he is the recipient of the 1997 ASME Materials Division Nadai Award for career achievement and the 2008 Khan International Medal for lifelong contributions to the field of metal plasticity. He currently serves on the editorial boards of several journals and is coeditor of the *International Journal of Fatigue*.

Series editor: Zhong Chen

Zhong Chen is a Professor in the School of Materials Science and Engineering, Nanyang Technological University, Singapore. In March 2000, he joined Nanyang Technological University (NTU), Singapore as an Assistant Professor and has since been promoted to Associate Professor and Professor in the School of Materials Science and Engineering. Since joining NTU, he has graduated 30 PhD students and 5 MEng students. He has also supervised over 200 undergraduate research projects (FYP, URECA, etc.). His research interest includes (1) coatings and engineered nanostructures for clean energy, environmental, microelectronic, and other functional surface applications and (2) mechanical behavior of materials, encompassing mechanics and fracture mechanics of bulk, composite and thin film materials, materials joining, and experimental and computational mechanics of materials. He has served as an editor/ editorial board member for eight academic journals. He has also served as a reviewer for more than 70 journals and a number of research funding agencies including the European Research Council (ERC). He is an author of over 300 peer-reviewed journal papers.

Elsevier Series in Mechanics of Advanced Materials

Uncertainty Quantification in Multiscale Materials Modeling

Edited by

Yan Wang and

David L. McDowell

Georgia Institute of Technology, Atlanta, GA, United States

WP
WOODHEAD PUBLISHING
An imprint of Elsevier

Woodhead Publishing is an imprint of Elsevier
The Officers' Mess Business Centre, Royston Road, Duxford, CB22 4QH, United Kingdom
50 Hampshire Street, 5th Floor, Cambridge, MA 02139, United States
The Boulevard, Langford Lane, Kidlington, OX5 1GB, United Kingdom

Notices

Knowledge and best practice in this field are constantly changing. As new research and experience broaden our understanding, changes in research methods, professional practices, or medical treatment may become necessary.

Practitioners and researchers must always rely on their own experience and knowledge in evaluating and using any information, methods, compounds, or experiments described herein. In using such information or methods they should be mindful of their own safety and the safety of others, including parties for whom they have a professional responsibility.

To the fullest extent of the law, neither the Publisher nor the authors, contributors, or editors, assume any liability for any injury and/or damage to persons or property as a matter of products liability, negligence or otherwise, or from any use or operation of any methods, products, instructions, or ideas contained in the material herein.

Library of Congress Cataloging-in-Publication Data
A catalog record for this book is available from the Library of Congress

British Library Cataloguing-in-Publication Data
A catalogue record for this book is available from the British Library

ISBN: 978-0-08-102941-1

Publisher: Matthew Deans
Acquisitions Editor: Dennis McGonagle
Editorial Project Manager: Ana Claudia A. Garcia
Production Project Manager: Swapna Srinivasan
Cover Designer: Matthew Limbert

Typeset by TNQ Technologies

Contents

Contributors

Ravi Agarwal Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign, Urbana, IL, United States

Jared A. Allison Mechanical Engineering Department, The University of Texas at Austin, Austin, TX, United States

Georgios Arampatzis Computational Science and Engineering Laboratory, ETH Zürich, Zürich, Switzerland

C. Bhave Department of Materials Science and Engineering, University of Florida, Gainesville, FL, United States

Thomas Bligaard SUNCAT Center for Interface Science and Catalysis, SLAC National Accelerator Laboratory, CA, United States

Ramin Bostanabad Department of Mechanical & Aerospace Engineering, University of California, Irvine, CA, United States

Brad L. Boyce Sandia National Laboratories, Albuquerque, NM, United States

Fabien Cailliez Laboratoire de Chimie Physique, CNRS, University Paris-Sud, Université Paris-Saclay, Orsay, France

Jian Cao Department of Mechanical Engineering, Northwestern University, Evanston, IL, United States

Wei Chen Department of Mechanical Engineering, Northwestern University, Evanston, IL, United States

Rune Christensen Department of Energy Conversion and Storage, Technical University of Denmark, Kongens Lyngby, Denmark

Amber D. Dressler Sandia National Laboratories, Albuquerque, NM, United States

John M. Emery Component Science and Mechanics Department, Sandia National Laboratories, Albuquerque, NM, United States

Baskar Ganapathysubramanian Department of Mechanical Engineering, Iowa State University, Ames, IA, United States

Ranjan Ganguli Department of Aerospace Engineering, Indian Institute of Science, Bangalore, India

Jiaying Gao Department of Mechanical Engineering, Northwestern University, Evanston, IL, United States

Mircea Grigoriu Civil and Environmental Engineering, Cornell University, Ithaca, NY, United States

Johann Guilleminot Department of Civil and Environmental Engineering, Duke University, Durham, NC, United States

Lijuan He-Bitoun Ford Motor Company, Dearborn, MI, United States

Karsten Wedel Jacobsen CAMD, Department of Physics, Technical University of Denmark, Kongens Lyngby, Denmark

Reese Jones Sandia National Laboratories, Livermore, CA, United States

Omar Knio King Abdullah University of Science and Technology, Thuwal, Saudi Arabia

Petros Koumoutsakos Computational Science and Engineering Laboratory, ETH Zürich, Zürich, Switzerland

Desiderio Kovar Mechanical Engineering Department, The University of Texas at Austin, Austin, TX, United States

Kurt Lejaeghere Center for Molecular Modeling (CMM), Ghent University, Zwijnaarde, Belgium

Yang Li Research & Advanced Engineering, Ford Motor Company, Dearborn, MI, United States

Biao Liang Department of Mechanical Engineering, Northwestern University, Evanston, IL, United States

Dehao Liu Woodruff School of Mechanical Engineering, Georgia Institute of Technology, Atlanta, GA, United States

Wing Kam Liu Department of Mechanical Engineering, Northwestern University, Evanston, IL, United States

Turab Lookman Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM, United States

David L. McDowell Georgia Institute of Technology, Atlanta, GA, United States

Pascal Pernot Laboratoire de Chimie Physique, CNRS, University Paris-Sud, Université Paris-Saclay, Orsay, France

Spencer Pfeifer Department of Mechanical Engineering, Iowa State University, Ames, IA, United States

Francesco Rizzi Sandia National Laboratories, Livermore, CA, United States

Balaji Sesha Sarath Pokuri Department of Mechanical Engineering, Iowa State University, Ames, IA, United States

Carolyn C. Seepersad Mechanical Engineering Department, The University of Texas at Austin, Austin, TX, United States

Xuming Su Research & Advanced Engineering, Ford Motor Company, Dearborn, MI, United States

Laura P. Swiler Optimization and Uncertainty Quantification Department, Sandia National Laboratories, Albuquerque, NM, United States

Aaron E. Tallman Los Alamos National Laboratory, Los Alamos, NM, United States

Yuan Tian State Key Laboratory for Mechanical Behavior of Materials, Xi'an Jiaotong University, Xi'an, Shaanxi, China

Michael R. Tonks Department of Materials Science and Engineering, University of Florida, Gainesville, FL, United States

Anh Tran Sandia National Laboratories, Albuquerque, NM, United States

Dallas R. Trinkle Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign, Urbana, IL, United States

Anton van Beek Department of Mechanical Engineering, Northwestern University, Evanston, IL, United States

Yan Wang Georgia Institute of Technology, Atlanta, GA, United States

Olga Wodo Department of Materials Design and Innovation, University at Buffalo, SUNY, Buffalo, NY, United States

X. Wu Department of Materials Science and Engineering, University of Florida, Gainesville, FL, United States

Dezhen Xue State Key Laboratory for Mechanical Behavior of Materials, Xi'an Jiaotong University, Xi'an, Shaanxi, China

Hongyi Xu Research & Advanced Engineering, Ford Motor Company, Dearborn, MI, United States

Ruihao Yuan State Key Laboratory for Mechanical Behavior of Materials, Xi'an Jiaotong University, Xi'an, Shaanxi, China

Danielle Zeng Research & Advanced Engineering, Ford Motor Company, Dearborn, MI, United States

Y. Zhang Department of Materials Science and Engineering, University of Florida, Gainesville, FL, United States

This page intentionally left blank

About the Series editors

Editor-in-Chief

Vadim V. Silberschmidt is Chair of Mechanics of Materials and Head of the Mechanics of Advanced Materials Research Group, Loughborough University, United Kingdom. He was appointed to the Chair of Mechanics of Materials at the Wolfson School of Mechanical and Manufacturing Engineering at Loughborough University, United Kingdom in 2000. Prior to this, he was a Senior Researcher at the Institute A for Mechanics at Technische Universität München in Germany. Educated in the USSR, he worked at the Institute of Continuous Media Mechanics and Institute for Geosciences [both—the USSR (later—Russian) Academy of Sciences]. In 1993−94, he worked as a visiting researcher, Fellow of the Alexander-von-Humboldt Foundation at Institute for Structure Mechanics DLR (German Aerospace Association), Braunschweig, Germany. In 2011−14, he was Associate Dean (Research). He is a Charted Engineer, Fellow of the Institution of Mechanical Engineers and Institute of Physics, where he also chaired Applied Mechanics Group in 2008−11. He serves as Editor-in-Chief (EiC) of the Elsevier book series on *Mechanics of Advanced Materials*. He is also EiC, associate editor, and/or serves on the board of a number of renowned journals. He has coauthored four research monographs and over 550 peer-reviewed scientific papers on mechanics and micromechanics of deformation, damage, and fracture in advanced materials under various conditions.

Series editors

David L. McDowell is Regents' Professor and Carter N. Paden, Jr. Distinguished Chair in Metals Processing at Georgia Tech University, United States. He joined Georgia Tech in 1983 and holds a dual appointment in the GWW School of Mechanical Engineering and the School of Materials Science and Engineering. He served as the Director of the Mechanical Properties Research Laboratory from 1992 to 2012. In 2012 he was named Founding Director of the Institute for Materials (IMat), one of Georgia Tech's Interdisciplinary Research Institutes charged with fostering an innovation ecosystem for research and education. He has served as Executive Director of IMat since 2013. His research focuses on nonlinear constitutive models for engineering materials, including cellular metallic materials, nonlinear and time-dependent fracture mechanics, finite strain inelasticity and defect field mechanics, distributed

damage evolution, constitutive relations, and microstructuresensitive computational approaches to deformation and damage of heterogeneous alloys, combined computational and experimental strategies for modeling high cycle fatigue in advanced engineering alloys, atomistic simulations of dislocation nucleation and mediation at grain boundaries, multiscale computational mechanics of materials ranging from atomistics to continuum, and system-based computational materials design. A Fellow of SES, ASM International, ASME, and AAM, he is the recipient of the 1997 ASME Materials Division Nadai Award for career achievement and the 2008 Khan International Medal for lifelong contributions to the field of metal plasticity. He currently serves on the editorial boards of several journals and is coeditor of the *International Journal of Fatigue*.

Thomas Böhlke is Professor and Chair of Continuum Mechanics at the Karlsruhe Institute of Technology (KIT), Germany. He previously held professorial positions at the University of Kassel and at the Otto-von-Guericke University, Magdeburg, Germany. His research interests include FE-based multiscale methods, homogenization of elastic, brittle-elastic, and visco-plastic material properties, mathematical description of microstructures, and localization and failure mechanisms. He has authored over 130 peer-reviewed papers and has authored or coauthored two monographs.

Zhong Chen is a Professor in the School of Materials Science and Engineering, Nanyang Technological University, Singapore. In March 2000, he joined Nanyang Technological University (NTU), Singapore as an Assistant Professor and has since been promoted to Associate Professor and Professor in the School of Materials Science and Engineering. Since joining NTU, he has graduated 30 PhD students and 5 MEng students. He has also supervised over 200 undergraduate research projects (FYP, URECA, etc.). His research interest includes (1) coatings and engineered nanostructures for clean energy, environmental, microelectronic, and other functional surface applications and (2) mechanical behavior of materials, encompassing mechanics and fracture mechanics of bulk, composite and thin film materials, materials joining, and experimental and computational mechanics of materials. He has served as an editor/editorial board member for eight academic journals. He has also served as a reviewer for more than 70 journals and a number of research funding agencies including the European Research Council (ERC). He is an author of over 300 peer-reviewed journal papers.

Preface

Human history shows evidence of epochs defined by new material discovery and deployment, which in turn have led to technology innovation and industrial revolutions. Discovery and development of new and improved materials has accelerated with the availability of computational modeling and simulation tools. Integrated Computational Materials Engineering has been widely pursued over the past decade to understand and establish the process−structure−property relationships of new materials. Yet the deployment of computational tools for materials discovery and design is limited by the reliability and robustness of simulation predictions owing to various sources of uncertainty.

This is an introductory book which presents various uncertainty quantification (UQ) methods and their applications to materials simulation at multiple scales. The latest research on UQ for materials modeling is introduced. The book reflects a range of perspectives on material UQ issues from over 50 researchers at universities and research laboratories worldwide. The target audience includes materials scientists and engineers who want to learn the basics of UQ methods, as well as statistical scientists and applied mathematicians who are interested in solving problems related to materials.

The book is organized as follows. Chapter 1 provides an overview of various UQ methods, both nonintrusive and intrusive, the sources of uncertainty in materials modeling, and the existing research work of UQ in materials simulation and design at different length scales. Chapters 2−5 describe the existing research efforts on model error quantification for quantum mechanical simulation to predict material properties via density functional theory. Chapters 6−7 provide state-of-the-art examples of Bayesian model calibration of interatomic potentials, the major source of errors in molecular dynamics simulation, and sensitivity analyses of their effects on physical property predictions. Chapters 8−10 provide examples of UQ methods developed for mesoscale simulations of materials, including kinetic Monte Carlo and phase field simulations. Chapters 11−13 discuss recent research of random fields and their applications to materials modeling in the higher length scale (mesoscopic) continuum regime, such as uncertainty propagation between scales in composites for mechanical property prediction and damage detection. Chapters 14 and 15 illustrate some of the unique UQ issues in multiscale materials modeling, including Bayesian model calibration based on information obtained from different scales, and reliability assessment based on stochastic reduced-order models with samples obtained using multifidelity simulations. Chapter 16 provides insight regarding materials design and optimization under uncertainty for cases in which Bayesian optimization and surrogate models can

play a major role. Chapter 17 highlights the challenges in metamaterial property and behavior predictions, where the variability induced by additive manufacturing processes needs to be quantified in simulations and incorporated in the material database.

We would like to thank all authors of the chapters for their contributions to this book and their efforts to advance the frontiers of the emerging field of UQ for materials. We are also in debt to our reviewers who rigorously examined the submissions, provided helpful feedback during manuscript selection, and improved the quality of the included chapters. This volume would not have been possible without the tireless efforts and devotion of Ms. Ana Claudia Abad Garcia, our Elsevier publishing editor and project manager, as well as the encouragement from the book series editor-in-chief Prof. Dr. Vadim Silberschmidt.

Yan Wang and David McDowell
Atlanta, Georgia, USA

Uncertainty quantification in materials modeling

1

Yan Wang, David L. McDowell
Georgia Institute of Technology, Atlanta, GA, United States

1.1 Materials design and modeling

New and improved materials have long fostered innovation. The discovery of new materials leads to new product concepts and manufacturing techniques. Historically, materials discovery emerges from exploratory research in which new chemical, physical, and biological properties of new materials become evident. Then their potential applications are identified. This discovery pathway is typically lengthy and has largely relied on serendipity. In contrast, intentional materials design is an application requirement−driven process to systematically search for solutions. In general, design involves iterative searching aimed at identifying optimal solutions in the design space, which is formed by the material composition and hierarchical structure (e.g., microstructure). The goal thus is to find compositions and structures that achieve the most suitable chemical and physical properties subject to various constraints, including cost, time, availability, manufacturability, and others.

A transformational trend in early 21st century is to incorporate computational modeling and simulation of material process−structure and structure−property relations to reduce materials development cycle time and its reliance on costly and time-consuming empirical methods. The Integrated Computational Materials Engineering (ICME) initiative [1,2] has been embraced by various industry sectors as a viable path forward to accelerate materials development and insertion into products by employing more comprehensive management of data, process monitoring, and integrated computational modeling and simulation. This has led more recently to the development of the US Materials Genome Initiative (MGI) [3], as well as companion thrusts in Europe and Asia [4], which aim to accelerate discovery and development of new and improved materials via a strategy of fusing information from experiments, theory, and computational simulation, aided by the tools of uncertainty quantification (UQ) and data science with the emphasis on high throughput protocols.

An accurate measurement to evaluate the role of ICME is the extent that it principally provides decision support for materials design and development. In other words, a metric for measuring the success of ICME is the increase of the fraction of decisions made in the critical path of materials development, optimization, certification, and deployment, where decision makers are informed via modeling and simulation as opposed to experiments. The same is true for the discovery of new materials as per objectives of the MGI.

Uncertainty Quantification in Multiscale Materials Modeling. https://doi.org/10.1016/B978-0-08-102941-1.00001-8

To design material systems [5] by tailoring the hierarchical material structure to deliver required performance requires that we go beyond the aims of basic science to explain phenomena and governing mechanisms, namely to understand and quantify these phenomena and mechanisms to the extent necessary to facilitate control and to manipulate structure at individual scales in a way that trends toward desired properties or responses. This change of emphasis toward connecting process to structure and structure to properties or responses undergirds much of the science base supporting ICME goals of materials design and development. The multiscale nature of material structure and responses is essential; multiscale modeling of utility to ICME must address the spatial- and temporal-scale hierarchies in order to

- Understand interaction mechanisms across length and time scales that affect cooperative properties arising from the hierarchical material structure;
- Improve materials by addressing both unit processes at fine scale and couplings of mechanisms across scales.

These two needs call for the application of systematic methods to search material structures and microstructures that deliver the required sets of properties or responses at various scales of interests. Multiscale modeling captures the responses and interactions of collective structures at various levels of material structure hierarchy. Further advances in multiscale modeling are necessary to understand the modes of materials synthesis in processing, as well as degradation or evolution in service.

Understanding the cause−effect relationship between material structure and properties or responses is a key element of materials design. The structure−property linkages can be regarded as "input−output" relations to facilitate engineering systems design of materials. Similarly, it is necessary to understand and quantify the relationship between fabrication and materials processing and resulting material structure. Physical realization of optimal material microstructures may be restricted by the limitations of available processing techniques. In many cases, available process−structure linkages are considered as constraints on accessible materials. As a result, the central task of materials design is to establish the process−structure−property (P−S−P) relationship based on the needs of properties or responses.

An example of P−S−P relationship is illustrated in Fig. 1.1 [6] for ultrahigh strength, corrosion-resistant steels. Each of the lines between boxes indicates a linkage from process to structure or from structure to property. We note that these mappings often involve phenomena that occur at multiple length and time scales, but these phenomena can manifest anywhere within the chain of P−S−P relations.

Modeling and simulation is an efficient means to augment physical experiments to identify P−S−P linkages. ICME tools at different scales have been developed to predict microstructures from fabrication processes and predict chemical and physical properties of microstructures. The major paradigm shift of ICME is to develop data-enhanced and simulation-based tools to inform decisions in materials design and development. However, there are tremendous challenges in predicting P−S−P relationships. The first challenge pertains to the quantitative representation of the hierarchical nature of material structures at various length scales. Advancement in multiscale computational modeling as required to bridge the length and time scale

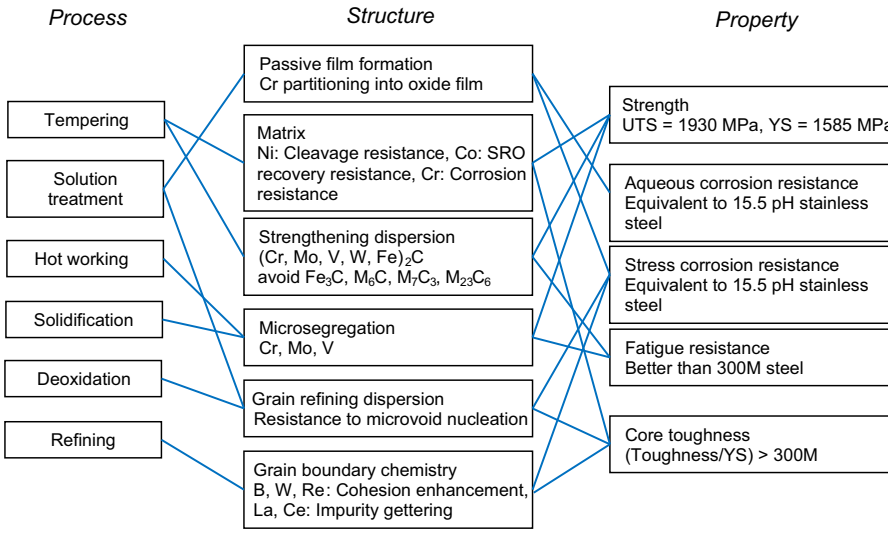


Figure 1.1 An example of process−structure−property relationship in designing ultrahigh strength, corrosion-resistant steels.
Adapted from G.B. Olson, Genomic materials design: the ferrous frontier. Acta Mater., 61(3) (2013) 771−781.

gaps is the second major challenge. The third challenge is the reliability and credibility of predictions from these models in the face of uncertainty from various sources.

The ultimate goal of ICME tools is to provide assistance to identify the P−S−P relationships and to inform decisions in materials selection and design processes under uncertainty. For centuries, uncertainty has been a key component underlying the domains of philosophy, mathematics, and statistical and physical sciences. The study of uncertainty led to a new branch of mathematics in the 17th century, known as probability. Although different interpretations of probability coexist and debates between scholars from these different schools persist for centuries, it has been generally accepted by all that the source of uncertainty is our lack of knowledge about future. In the domains of physical sciences, two sources of uncertainty are differentiated. One is the lack of perfect knowledge and the other is the random fluctuation associated with finite temperature processes. The former is referred to by many as *epistemic*, whereas the latter is *aleatory*. Any uncertainty phenomenon we observe is the conflated effect of these two components. The differentiation of these two components is pragmatic and mainly for decision-making practitioners. Epistemic uncertainty often appears as bias or systematic error in data or simulation results and is regarded as reducible; increasing our level of knowledge can reduce the epistemic component of uncertainty. In contrast, aleatory uncertainty appears as random error and is irreducible. Random fluctuation inherently exists in position of atoms and electrons at temperatures above absolute zero and is manifested as uncertainty of material structure at various scales. When decision makers can differentiate the sources of uncertainty,

the risk of a go/no-go decision is more readily managed. Gaining more knowledge to reduce the epistemic component of uncertainty will generally lead to more precise estimation of the risk.

ICME tools, such as density functional theory (DFT), molecular dynamics (MD), coarse-graining atomistic modeling methods, kinetic Monte Carlo (kMC), dislocation dynamics (DD), microscopic and mesoscopic phase field (PF), and finite-element analysis (FEA), predict physical phenomena at different length and time scales. The sources of uncertainty associated with these tools should be identified if we would like to make robust decisions based on the results of these computational tools.

All models require certain levels of abstraction. Simplification can be related to dimensional reduction in parameter space when too many factors are involved, separation of size or time scales, and separation of physical domains when tightly coupled physics confers complexity to models. Assumptions of independence between factors, temporally or spatially, are often made to reduce model complexity. Approximation error is always involved, and truncation is inevitable when functional analysis is applied in modeling and experimental data analysis. Numerical discretization or linearization is regularly applied during computation. Furthermore, the choice of model forms from domain experts is typically subjective and based on user preference. The subjectivity of model choice also includes the unintended bias or convenient shortcuts in the modeling process of each expert based on their own scope of knowledge and understanding. As a result of simplification, approximation, and subjectivity, all models have *model form uncertainty* and it affects the predictions.

In addition, the parameters of models need to be calibrated for accurate prediction. Calibration-related model errors are called *parameter uncertainty*. Typically, model predictions are compared with experimental observations, and the parameters are adjusted to match with the observations. Data fitting or optimization procedures are pursued in the calibration process. All experimental measurements have systematic errors stemming from instruments or human operators. This leads to bias in the parameters of the fitted empirical model. Random errors from experimental measurements, especially with a small dataset, are also propagated to models. All sensors that are used to collect data rely on certain mathematical or physical models to map the collected signals to quantities of interest. These sensor models also have model form and parameter uncertainties. These errors associated with the underlying sensor models are in turn propagated to the models that are being calibrated. In first principles modeling, model parameters are calibrated based on first principles calculations and seek consistency with higher scale observations. The model form and parameter uncertainties of the first principles models also propagate through model calibration.

Model form uncertainty and parameter uncertainty are the major components of epistemic uncertainty. An overview of model form and parameter uncertainties in multiscale modeling is listed in Table 1.1. Lack of perfect knowledge about the physical phenomena also contributes to the discrepancy between the models and actual physics. Needless to say, bias also exists in the data archived in ICME databases that are produced either via experiment or simulation [7].

Model form and parameter uncertainties affect the accuracy of the predictions of ICME tools. The reliability of P−S−P linkages can be problematic. The errors

Table 1.1 An overview of model form and parameter uncertainties in multiscale modeling.

Category	Source	Examples
Model form uncertainty	Simplification	Dimension reduction Separation of scales Separation of physics Independence assumption
	Approximation	Truncation Numerical treatment
	Subjectivity	Model preference Knowledge limitation
Parameter uncertainty	Experiment data	Systematic error Random error Sensor model
	First principles models	Model form uncertainty Parameter uncertainty

associated with the predictions need to be quantified so that the robustness of design can be assessed. UQ is the exercise of applying quantitative methods to measure and predict uncertainty associated with experimental data and model predictions. The predicted uncertainty is used to support risk analysis and decision making in materials design and development. Various UQ methods, including probabilistic and nonprobabilistic approaches, have been developed in the areas of statistics and applied mathematics and have been widely applied in engineering and science domains. Uncertainty is usually quantified in terms of probability distributions, confidence intervals, or interval ranges. In modeling and simulation, uncertainty is associated with model inputs, e.g., initial and boundary conditions, which comes from the sources of data. Uncertainty propagates to the output of simulation, spatially and temporally, confounded with model form and parameter uncertainties associated with the simulation model(s).

It is particularly challenging to estimate uncertainty propagation in UQ methods for materials modeling because materials modeling often relies on application of multiple tools at different length and time scales that range from discrete to continuous, with a large number of design variables. Formal application of model order reduction concepts across these disparate models differs substantially from traditional applications of continuum modeling for solids and fluids where the discrete character of defects and structures that controls responses of materials at fine scales is not considered. Reduced-order models themselves introduce model-form errors. Traditional stochastic modeling is typically confined to a single class of models with a given set of governing differential equations to address parametric uncertainty associated with variability of fields. Each simulation tool, such as DFT, MD, kMC, DD, PF,

and FEA, has a unique basis and set of assumptions and is limited to a particular range of length and time scales. Given the hierarchical nature of materials, sufficient understanding of material behavior often requires multiple tools to be applied. The outputs of a lower scale model are usually used as inputs to a higher scale model, whether operating sequentially (hierarchical modeling) or concurrently. Moreover, materials often exhibit a very strong sensitivity of response to change of configuration of structure and/or defects that is not smooth and continuous, which challenge the coarse-graining and model order reduction approaches that attempt to address material response over many length and perhaps time scales. Hence, propagation of uncertainty arises not only from individual scales in the hierarchy of material structure but also from the way in which information from different models is interpreted to inform the application of models at other scales (so-called scale-bridging or linking). Cross-scale propagation is one of the unique issues in UQ for materials modeling.

The purpose of this first chapter is to provide an overview of the sources of uncertainty in materials modeling, as well as the major classes of UQ methods that have been developed in the past few decades. As the ICME paradigm is adopted by researchers in materials science and engineering, understanding the sources of uncertainty in materials modeling and choosing appropriate UQ methods to assess the reliability of ICME prediction become important in materials design and development, as well as in deployment of materials into products.

1.2 Sources of uncertainty in multiscale materials modeling

We focus here on uncertainty in materials modeling across length and time scales. Reliable simulation requires that uncertainty to be quantified and managed. The first step of UQ is to identify the sources of uncertainty in the model. Based on the sources, epistemic and aleatory components of uncertainty are differentiated. The differentiation is helpful for us to apply different quantification and management strategies to the two components. For the epistemic component, which is due to the lack of knowledge, increasing the level of knowledge about the system under study can help reduce the uncertainty. Examples of strategies to reduce epistemic uncertainty include (i) building a more accurate physical model with better understanding of the physics and cause−effect relationships, (ii) controlling the most sensitive factors that cause the variations in model predictions or experimental observations, (iii) performing model calibration with a larger amount of data collection for targeted sensitive parameters, and (iv) conducting instrument calibration based on more precise standard references to reduce the systematic error. In contrast to epistemic uncertainty, aleatory uncertainty owes to the inherent randomness due to fluctuation and perturbation, which cannot be reduced. To cope with it, we typically perform multiple measurements or multiple runs of simulations and use the average values, with the notion of variance, to predict the true but unknown quantities of interest subject to variability.

1.2.1 Sources of epistemic uncertainty in modeling and simulation

The major sources of epistemic uncertainty in the general scheme of modeling and simulation are illustrated in Fig. 1.2, which can be categorized as data related and model related. They are summarized as follows.

The data-related epistemic uncertainty is due to

- Lack of data or missing data. The parameters of models, probability distributions, and distribution types are uncertain when the sample size is small. The availability of high-quality experimental data is critical for fitting data during model calibration and for comparison in model validation. In materials modeling, the additional challenge is that it may not be possible to directly measure the quantity of interest (QoI) because of experimental techniques. A different quantity, sometime at a different scale, is measured and used to infer the value of the QoI. Lack of sufficient information will introduce errors in models and requires the analyst to find new ways to describe the associated uncertainty more rigorously.
- Measurement errors. Systematic errors can be introduced because of the limitation of measurement environment, measurement procedure, and human error. In addition, most sensing protocols in measurements rely on some type of sensor models that relate QoIs to electrical signals. Model form and parameter uncertainty associated with these sensor models also contribute to measurement error.

The model-related epistemic uncertainty is due to

- Conflicting information. If there are multiple sources of information, the analyst may face conflicts among them in model selection. For instance, it is not appropriate to draw a simple conclusion regarding distributions from several pieces of contradictory evidence. The inconsistency results in potentially inaccurate types of distributions.

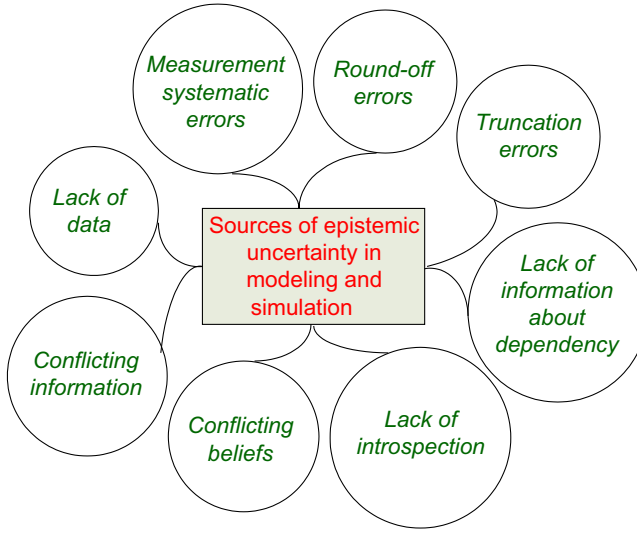


Figure 1.2 Major sources of epistemic uncertainty in modeling and simulation.

- Conflicting beliefs. When data are not available or are limited, the analyst usually relies on expert opinions and beliefs to determine the model forms. Information obtained from the experts is subjective due to the diversity of their past experiences and their own understanding of relevant phenomena, which can easily lead to inconsistent model predictions. This is particularly true of assigning phenomena to consider in multiscale modeling and can arise from differing perspectives of materials science and structural mechanics communities, for example.
- Lack of introspection. In some cases, the analyst cannot afford the necessary time to think deliberately about an uncertain process or event, derive more accurate description of physical systems, perform more sensitivity studies, or run additional simulations. The lack of introspection increases the risk of using inaccurate model.
- Lack of information regarding dependencies. Given the limitation of modeling and simulation techniques, a complex system is usually decomposed into subsystems, which are assumed to be independent from each other to mitigate complexity. Lack of knowledge about the correlations among factors and variables, as well as unknown time dependency of these factors, contribute to the error and bias in model predictions.
- Truncation errors. Functional analysis is the foundation for modeling and simulation which enables numerical methods to solve differential equations and model stochastic processes. It is also widely applied in spectral analysis of experimental data. Truncation is inevitably applied in the analysis for affordable computational expenses.
- Round-off errors. Floating-point representation is essential for digital computers to represent real numbers. The errors can become prominent when the number of arithmetic operations increases, e.g., system dynamics simulation with a very short time step but for a long period of time.

In modeling and simulation, epistemic uncertainty is the result of the errors mainly associated with the models and input data. Since aleatory and epistemic uncertainties stem from separate sources and have very different characteristics, they are ideally distinguished and modeled in different forms. Aleatory uncertainty is traditionally and predominantly modeled using probability distributions. Epistemic uncertainty however has been modeled in several ways, including probability, interval or convex bounds, random sets, etc.

1.2.2 Sources of model form and parameter uncertainties in multiscale models

1.2.2.1 Models at different length and time scales

Model form and parameter uncertainties are major epistemic components of error in modeling and simulation. These are elaborated next in commonly used ICME materials modeling tools at various scales.

In DFT simulations, the major source of model form uncertainty is the exchange-correlation potential functionals, where many-particle interactions are approximated and simplified in the data fitting procedure. The so-called rungs in Jacob's ladder, varying from local spin-density approximation to generalized gradient approximation (GGA), meta-GGA, hyper-GGA, and higher-order approximations, lead to different accuracy levels. In addition, the Born-Oppenheimer approximation assumes that the

lighter electrons adjust adiabatically to the motion of the heavier atomic nuclei, and thus their motions can be separated. Zero-temperature ground state of the system is also assumed in DFT calculation. In addition, the pseudopotentials are typically used to replace the Coulomb potential near each nucleus in the calculation to reduce computational load, which also introduces approximation error. Error is also introduced in the trade-offs between long-range and short-range dispersions and between efficiency and accuracy during the approximation. Numerical treatments such as k-point sampling and orbital basis selection also introduce model form uncertainty. In the self-consistent calculation of ground state energy, the chosen threshold for convergence introduces additional numerical errors.

In MD simulations, the major sources of model form and parameter uncertainty are associated with the interatomic potential functions, most of which are obtained empirically. The choice of analytical forms, number of parameters, and the calibration process introduce approximation errors. The systematic error in measurement data can be inherited through calibration. The errors associated with the interatomic potentials propagate to the output prediction through the simulation process. Prediction errors of extrapolative nature emerge when interatomic potentials are calibrated with one property but used to predict another property. Other sources of uncertainty include the cut-off distance in simulation for ease of computation, the type of imposed boundary conditions (e.g., periodic) that may introduce artificial effects, small simulation domain size that is not representative of realistic defect structures and may lead to image stresses, deviation of microstructure from the physical case, and use of short simulation times to estimate statistical ensemble behavior. To overcome the time scale limitation of MD, errors are introduced in accelerating simulations by use of larger time steps, modified interatomic potentials to simulate transitions, high temperatures, parallel replicates for rare events, or the application of physically unrealistic high strain rates due to mechanical and/or thermal loading. Computational errors with different computer architectures arise due to round-off in floating-point numbers as well as task distribution and sequencing in parallel computation.

In kMC simulation, the major sources of epistemic uncertainty are incomplete event catalogs and imprecise associated rates or propensities. The accuracy of kMC simulation depends on the validity of complete knowledge of all possible events, which is impossible. Furthermore, the actual kinetic rates can vary with time. They also depend on the state of the system. For instance, external loads can alter the diffusion of defects. The crowding effect reduces reaction rates when molecules or reaction products block reaction channels. The assumption of constant rates is unreasonable in such cases. In kMC, events are also assumed to be independent from each other, and the interarrival times between events are assumed as random variables that follow exponential distributions. These assumptions simplify computation. In reality, the events may be correlated, and memory effects in evolution of material structure also violate the assumption of exponential distributions. These assumptions and simplifications lead to model form uncertainty, in addition to parameter uncertainty arising from calibration with experimental data.

In discrete DD simulation models, the major approximations include the modeling of the stress field and phenomenological rules for dislocation−dislocation interactions,

neglect of dislocation core spreading and partial dislocations, interactions of dislocations with precipitates or other second phases, and interfaces. Simple mobility relations are assumed with considerable uncertainty. Numerical errors are introduced with the piecewise linear approximations of dislocation curves during discretization, and numerical solutions of ordinary differential equations. Similarly, in continuous DD simulations, the major sources of uncertainty include the approximation of dislocation density evolution with the associated partial differential equations over ensembles. Numerical errors are introduced in the solving process based on spectral analysis with truncation and calculating integrals.

In PF simulation, the major source of model form and parameter uncertainty is the empirical model of the free energy functional, which is usually derived from principles of thermodynamics with assumptions of constant temperature, pressure, or volume, with approximation errors from truncation and pure empirical data fitting. The additional numerical treatment in solving the partial differential equations of Cahn–Hilliard and Allen–Cahn also introduces errors. This includes the antitrapping current to eliminate the solution trapping during interface diffusion when an interface larger than the physical one is modeled in order to improve computational efficiency. Some other parameter uncertainty is caused by assumptions such as temperature-independent interface mobility and location-independent diffusion coefficient.

In FEA simulations, besides the model form uncertainty inherited in partial differential equations and material constitutive laws, approximation errors are the result of domain discretization with meshes, interpolation with limited numbers of basis functions, truncation with low-order approximations, numerical methods to solve linear equations, and others.

In summary, incomplete description of physics, experimental data, and numerical treatment introduce epistemic uncertainty into simulation models. As a result, the prediction of QoI as the simulation output is inherently inaccurate. When QoIs are statistical ensembles that depend on temperature, the output is also imprecise and contains variability. Therefore, the simulation output usually contains the confounded effects of model form, parameter, and aleatory uncertainties.

1.2.3 Linking models across scales

UQ for ICME has the distinct need to consider uncertainty propagation between multiple length and time scales in material systems. Uncertainty observed at a larger scale is the manifestation of the collective uncertainties exhibited at smaller scales. For instance, the nondeterministic strengths of material specimens are due to the statistical distributions of grain boundaries and defects. The randomness of molecular movement known as Brownian motion arises from the stochasticity of physical forces and interactions among electrons at the quantum level. The ability to model the propagation of uncertainty between scales is essential to obtain useful information from multiscale modeling as necessary to inform understanding of higher-scale material response and to support decision making in materials design and development. Existing ICME tools simulate material systems over a range from nanometers to micrometers. The major challenge of UQ in these tools is the information exchange between

different models, where assumptions of scales and boundaries are made a priori. For purposes of model validation, not all physical quantities predicted in simulation can be directly observed, especially those at small length and short time scales. Measurable quantities at larger scales are typically used to validate models. This is based on some assumed, implied, and/or derived correlation between measured quantities and unobservable quantities, which introduces model form uncertainty as part of sensing or measurement errors. In other words, even physical measurements appeal to some model construct to interpret. As a result, model calibration and model validation face new challenges in multiscale modeling.

Another pervasive and understated challenge for multiscale materials modeling is the common lack of "smoothness" between material response functions and microstructure. The structure−property relationships can be highly nonlinear. For example, phase transformations confer distinct jumps of structure and properties. Moreover, the nature of the interaction of defects with interfaces in crystals depends substantially on the structure of the interface and character of the applied stress state. Strong temperature dependencies in kinetics of evolution can lead to evolution of local microstructure states that differ from assumed isothermal conditions. In many cases, applications involving uncertainty propagation in mechanics of structures based on finite-element modeling, for example, do not address these kinds of common, material-specific nonlinearity or discontinuities in material structure evolution and associated responses. Such cases require the identification of these complex mechanisms, in addition to a multifidelity modeling capability capable of resolving or addressing them.

This latter point brings us to a distinction between so-called hierarchical and concurrent multiscale modeling [8]. Models pertaining to different levels of the material structure hierarchy are typically related to each other or exercised in one of two ways: hierarchical (one-way, bottom up) or concurrent (two-way) multiscale schemes. *Concurrent multiscale modeling* schemes exercise simultaneous simulations for models with different fidelities or spatial resolutions over the same temporal duration, necessitated in cases where (i) time scales are not separable for phenomena that occur at several length scales of interest or (ii) the collective, higher-scale responses of interest relate inextricably to certain fine-scale features or mechanisms that differ from one problem to the next. An example is a specific type of failure mechanism solicited by a specific higher-scale component geometry (e.g., notch) or loading condition (e.g., low velocity impact). These models can be either applied to the same spatial domain with different spatial resolution and degrees of freedom or pursued with different fidelity in adjacent, abutting, or overlapping domains; the latter requires schemes for communication of model responses between these regions and are typically referred to as domain decomposition methods. *Hierarchical multiscale modeling schemes* typically pass information from models exercised at each successive length and/or time scale to the next higher scale(s), with the intent to instruct model form and/or parameters of the latter. In some cases, they can pass information to models framed at much higher scales. For example, elastic constants and diffusion coefficients computed using DFT or other atomistic simulations can be employed in crystal plasticity models or macroscale plasticity models. They may be hierarchical in length and time, adding additional flexibility to the framing of the multiscale modeling problem. Most

multiscale modeling work to date has focused more on hierarchical multiscale models that are linked by handshaking or passing of information from the outputs of one model to the inputs of the next. Formulation of concurrent multiscale models, particularly for a heterogeneous set of models at various scales, is quite challenging if there is an attempt to identify and track the sources of uncertainty.

As another special challenge of UQ in multiscale modeling, uncertainty propagation between scales needs to be carefully treated. Simply regarding these models as series of "black boxes" with simple input−output functional relations has the tendency to overestimate uncertainty. The QoIs between scales are intrinsically correlated. As a result, uncertainty is not necessarily always worsened or amplified through propagation. Understanding of the physics assists to more accurately estimate uncertainty.

1.3 Uncertainty quantification methods

Various UQ methods have been developed in the past half century. Most UQ approaches have been based on probability theory. Alternative approaches [9] such as evidence theory, possibility, interval analysis, and interval probability have also been developed, differentiating between aleatory and epistemic uncertainty. With respect to the application of modeling and simulation, UQ methods can be categorized as either intrusive or nonintrusive. Nonintrusive UQ methods do not require an internal representation of uncertainty in the simulation models. The original simulation tools are treated as "black boxes" and the UQ methods are implemented as parent processes to call upon the simulation tools to conduct the necessary evaluations. In contrast, intrusive UQ methods require the modification of the original simulation software tools so that uncertainty can be represented internally. This distinction is very important in light of the nature of hierarchy of length and time scales in the heterogeneous cascade of multiscale models. Specifically, intrusive methods require that uncertainty propagates internal to the entire system of models, including linking formalisms between models; this is quite challenging in view of the need to adaptively refine and make decisions regarding treatment of scales within each of the distinct models. Nonintrusive methods might be attractive in such cases owing to their more modular character in assisting to construct flexible workflows; however, they likely do not scale well for solving high-dimensional problems and the implementation in high-performance computing architectures.

Commonly used nonintrusive UQ methods include Monte Carlo (MC) simulation, global sensitivity analysis (GSA), surrogate models, polynomial chaos, and stochastic collocation. Common intrusive UQ methods include local sensitivity analysis (LSA), stochastic Galerkin, and interval-based approaches.

1.3.1 Monte Carlo simulation

MC simulation is the earliest formal attempt to quantify uncertainty inherent in physical models, where pseudo random numbers are generated by computers and used in

evaluating models, although the technique was originally devised to numerically calculate deterministic integrals in quantum mechanics (with its inherent uncertainty). The effectiveness of MC relies on how truly "random" the numbers generated by the pseudo random number generators (PRNGs) are. Common implementations of PRNGs as the core of MC to generate uniformly distributed numbers include linear congruential method [10,11] and its various extensions [12−16] for longer periods and better uniformity, feedback shift register generators [17,18], and Mersenne twister [19]. Based on the uniformly distributed numbers, random variates that follow other distributions can be generated via computational methods such as inverse transform, composition, convolution, and acceptance−rejection. When MC is applied to assess the uncertainty associated with the inputs of a model, inputs with predetermined distributions are randomly generated. They are used to evaluate the model or run the simulation many times. The distribution of the resulting outputs is then used to assess the effect of uncertainty, which is quantified with statistical moments of different orders.

The major issue with MC for UQ in ICME is its computational cost. The quality of uncertainty assessment depends on how many runs of simulation can be conducted in order to generate statistical distributions of outputs and draw meaningful conclusions from the results. Worse yet, for a high-dimensional sampling space where many input variables are involved, the number of samples to densely cover the sampling space grows exponentially as the dimension increases. If each simulation run is expensive, as is the case with DFT and MD and with higher scale models that explicitly address 3D microstructure, the cost of UQ will be high in the pure sampling−based approach. In addition, MC also requires predetermined input distributions from which the samples are drawn.

If there is a lack of prior knowledge regarding the types of distribution types or lack of experimental data, the effect of model form uncertainty needs to be assessed. Second-order Monte Carlo (SOMC) [20,21] is a natural extension of MC to study the uncertainty associated with the input distributions. In the outer loop, the parameters or types of statistical distributions are randomly sampled. In the inner loop, classical MC is applied with each of the sampled distributions to study the variability. The SOMC results can provide an overall picture of the combined effects from both epistemic and aleatory uncertainties.

1.3.2 Global sensitivity analysis

Sensitivity analysis is a general concept of studying how uncertainty in the output of a model is attributed to uncertainty associated with model inputs. GSA [22] quantifies the effect of each individual input as well as their joint effects by conducting the analysis of variance.

For a given model or simulation input−output relation $Y = f(X_1, \ldots, X_n)$ where input X_i's are random variables, by fixing input variable X_i to be x_i^* one at a time, the conditional variance of the output $Var\left(Y \middle| X_i = x_i^*\right)$ is typically less than the original total variance $Var(Y)$. The difference between the two is an indicator of the contribution of variance from input variable X_i, i.e., the sensitivity of output uncertainty with

respect to input X_i. Given all possible values of x_i^*, $Var\left(Y\middle|X_i = x_i^*\right)$ itself is a random variable. Thus, its expected value $\mathbb{E}[Var(Y|X_i)]$ can be calculated. The deterministic value $Var(Y) - \mathbb{E}[Var(Y|X_i)]$ therefore is a metric to quantify the importance of input X_i. Similarly, the conditional expectation $\mathbb{E}\left[Y\middle|X_i = x_i^*\right]$ with all possible values of x_i^* is a random variable. Equivalently, the value $Var(Y) - Var(\mathbb{E}[Y|X_i])$ is an indicator of the contribution of variance from input variable X_i, because $Var(Y) = \mathbb{E}[Var(Y|X_i)] + Var(\mathbb{E}[Y|X_i])$. The first-order Sobol' sensitivity index [23,24] $S_i = Var(\mathbb{E}[Y|X_i])/Var(Y)$ is commonly used to quantify the sensitivity of output with respect to the uncertainty associated with the ith input variable, which is referred to as the main effect. The interactions among input variables are estimated by second- or higher-order sensitivity indices. By fixing two variables X_i and X_j simultaneously at a time, $Var(\mathbb{E}[Y|X_i, X_j])$ measures the joint effect of the two variables. The second-order index $S_{ij} = Var(\mathbb{E}[Y|X_i, X_j])/Var(Y) - S_i - S_j$ shows the interaction effect of the two input variables.

Higher-order indices can be defined in a similar way. In general, the total variance can be decomposed as $Var(Y) = \sum_i V_i + \sum_{i,j>i} V_{ij} + \sum_{i,j>i,k>j} V_{ijk} + \ldots + V_{1,2,\ \ldots\ ,n}$ where $V_i = Var(\mathbb{E}[Y|X_i])$, $V_{ij} = Var(\mathbb{E}[Y|X_i, X_j]) - V_i - V_j$, $V_{ijk} = Var(\mathbb{E}[Y|X_i, X_j, X_k]) - V_{ij} - V_{jk} - V_{ik} - V_i - V_j - V_k$, etc. Therefore, $\sum_i S_i + \sum_{i,j>i} S_{ij} + \sum_{i,j>i,k>j} S_{ijk} + \ldots + S_{1,2,\ \ldots\ ,n} = 1$. The total effect of X_i, including all orders that have X_i involved, is measured by the total effect index [25] $S_{Ti} = 1 - \sum_{j \neq i} S_j - \sum_{j,k>j, j \neq i} S_{jk} - \ldots = 1 - Var(\mathbb{E}[Y|X_1, \ldots, X_{i-1}, X_{i+1}, \ldots, X_n])/Var(Y)$. Using the latter approach to calculate the total effect index is computationally more tractable.

It should be noted that variance-based GSA does not require a known or closed-form mathematical function $Y = f(X_1, \ldots, X_n)$ for the input−output relation. For black-box simulations, if enough runs of simulations are conducted with proper design of experiments to generate statistically meaningful pairs of input and output, GSA can be performed by the analysis of variance. Instead of variance, other moment-independent sensitivity indices [26,27] have also been proposed to directly quantify the importance of input uncertainty based on cumulative distributions or density functions.

The limitation of GSA for ICME applications is similar to the one in MC, since MC sampling is typically needed to estimate the variances. Notice that traditional MC only provides information regarding overall output distributions, whereas GSA can provide fine-grained information of individual and compounded effects of input variables. Instead of variance, other measures of uncertainty can also be applied for GSA, such as the Hartley-like measure [28] which quantifies the level of uncertainty by the width of an interval range. This approach can avoid the high computational cost of sampling in variance-based GSA.

1.3.3 Surrogate modeling

When the input−output relations in simulation models are too complex, expensive, or unknown, surrogate models can be constructed to approximate the response between inputs and outputs. The simplified surrogate models, typically in the form of polynomials or exponentials, can improve the efficiency of model evaluations and predictions. For UQ, surrogate models can be used for sensitivity analysis and prediction of response variation. The input−output responses can be generated by experimental designs such as factorial, fractional factorial, central composite, and orthogonal designs [29−31]. The resulting models are generally called response surfaces. They are constructed by interpolation or regression analysis of the results from simulations with combinations of input variable values. With the constructed response surfaces, performance of new input values and the sensitivity can be predicted without running the actual simulation itself.

To construct response surfaces, sampling the input parameter space thoroughly is important because predictions from interpolation are generally more reliable than those from extrapolation. For high-dimensional input parameter space, exhaustive sampling with all possible combinations can be very costly. The computational complexity grows exponentially as the dimension increases. Latin hypercube sampling (LHS) [32−34] is an efficient sampling approach to choose samples in high-dimensional space. It is a stratified sampling strategy for variance reduction where samples are taken from the predefined input subspaces. For each subspace, there is an equal probability that the input samples are drawn from. The sampling is then performed within each of these subspaces so that all subspaces can be covered by much fewer samples than classical MC sampling. Thus, the number of samples can be significantly reduced while results are still statistically representative. LHS is also extended to dividing subspaces with unequal probabilities, and the estimates are weighted by the corresponding probability values [35]. LHS is a versatile tool and can be applied to study statistical properties of responses directly without constructing response surfaces. The limitation of LHS is that the efficiency of the sampling strategy depends on the prior knowledge of probability distributions associated with input variables. When there is a lack of knowledge about the types and parameters, the variance reduction technique may introduce bias.

1.3.4 Gaussian process regression

Kriging or Gaussian process regression [36,37] is a regularized regression approach to find approximated response models between inputs and outputs. It predicts new functional value from some existing ones by modeling the underlying but unknown true function as a Gaussian process. Different from simple regression with the point estimation of model parameters, the probability distributions of model parameters are estimated. Gaussian process can be regarded a special type of stochastic process

which is only specified by the mean vector and covariance matrix. The modeling and prediction are based on Bayesian inference. That is, given the prior probability $P(M_\alpha)$ for different models M_α ($\alpha = 1, 2, \ldots$), as well as the likelihood $P(D|M_\alpha)$ associated with observation D, the posterior probability of M_α is obtained as $P(M_\alpha|D) \propto P(D|M_\alpha)P(M_\alpha)$. The prediction of a new value y is the Bayesian model average, calculated as

$$P(y) = \sum_\alpha P(y|M_\alpha)P(M_\alpha|D) \tag{1.1}$$

The major assumption in Gaussian process regression is that the functional values for existing inputs follow a joint Gaussian distribution. As a result, the prediction of the new value is simplified to be the weighted average of the existing values plus an additive noise as a stationary covariance process with zero mean. This is illustrated with the following example of generalized linear regression. A Gaussian process is specified by a mean function $\mu(\boldsymbol{x}) = \mathbb{E}[Y(\boldsymbol{x})]$ and a covariance function $\mathbb{C}(Y(\boldsymbol{x}), Y(\boldsymbol{x}')) = k(\boldsymbol{x}, \boldsymbol{x}')$. Based on a finite set of basis functions $\{\phi_j(\boldsymbol{x}), j = 1, \ldots, m\}$, the output function is expressed as

$$Y(\boldsymbol{x}) = \sum_{j=1}^{m} w_j \phi_j(\boldsymbol{x}) + \varepsilon = \boldsymbol{\phi}(\boldsymbol{x})^{\mathrm{T}} \boldsymbol{w} + \varepsilon = y(\boldsymbol{x}; \boldsymbol{w}) + \varepsilon \tag{1.2}$$

where $\boldsymbol{w} = [w_1, \ldots, w_m]^{\mathrm{T}}$ is the weight vector, $\boldsymbol{\phi}(\boldsymbol{x}) = [\phi_1(\boldsymbol{x}), \ldots, \phi_m(\boldsymbol{x})]^{\mathrm{T}}$ is the vector of basis functions, and Gaussian noise $\varepsilon \sim N(0, \sigma_0^2)$ is assumed to be associated with observations. Let the prior probability distribution of the weight vector $\boldsymbol{w}$ be Gaussian $N(0, \boldsymbol{\Sigma}_w)$, as

$$P(\boldsymbol{w}) = \frac{1}{(2\pi)^{m/2} |\boldsymbol{\Sigma}_w|^{1/2}} \exp\left(-\frac{1}{2} \boldsymbol{w}^{\mathrm{T}} \boldsymbol{\Sigma}_w^{-1} \boldsymbol{w} \right) \tag{1.3}$$

With the observed dataset $D = \{(\boldsymbol{x}_i, y_i), i = 1, \ldots, n\}$ with n input−output tuples and independent observation assumption, the likelihood is

$$P(y_1, \ldots, y_n|\boldsymbol{w}) = \frac{1}{\left(2\pi\sigma_0^2\right)^{n/2}} \prod_{i=1}^{n} \exp\left(-\frac{1}{2\sigma_0^2} (y_i - y(\boldsymbol{x}_i; \boldsymbol{w}))^2 \right) \tag{1.4}$$

based on the Gaussian kernel $k(\boldsymbol{x}, \boldsymbol{x}') = \exp\left(-\frac{1}{2\sigma_0^2} |\boldsymbol{x} - \boldsymbol{x}'|^2 \right)$. The posterior mean value of weights $\widehat{\boldsymbol{w}}$ is obtained by minimizing the negative logarithmic of the posterior probability, as

$$\min_{\boldsymbol{w}} E(\boldsymbol{w}) = \min_{\boldsymbol{w}} \frac{1}{2\sigma_0^2} \sum_{i=1}^{n} \left(y_i - \boldsymbol{w}^{\mathrm{T}} \boldsymbol{\phi}(\boldsymbol{x}_i) \right)^2 + \frac{1}{2} \boldsymbol{w}^{\mathrm{T}} \boldsymbol{\Sigma}_w^{-1} \boldsymbol{w} \tag{1.5}$$

By solving the linear equations $\partial E/\partial \boldsymbol{w} = 0$, we obtain

$$\widehat{\boldsymbol{w}} = \sigma_0^{-2}\mathbf{A}^{-1}\boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{y} \tag{1.6}$$

where $\boldsymbol{y} = [y_1, \ldots, y_n]^{\mathrm{T}}$ is the vector of observations, matrix $\mathbf{A} = \boldsymbol{\Sigma}_w^{-1} + \sigma_0^{-2}\boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{\Phi}$, and $\boldsymbol{\Phi}$ is the $n \times m$ design matrix with elements $\phi_j(\boldsymbol{x}_i)$'s. For a new input $\boldsymbol{x}_*$, the predicted mean function value is

$$\begin{aligned}\mathbb{E}[Y(\boldsymbol{x}_*)] = \boldsymbol{\phi}(\boldsymbol{x}_*)^{\mathrm{T}}\widehat{\boldsymbol{w}} &= \sigma_0^{-2}\boldsymbol{\phi}(\boldsymbol{x}_*)^{\mathrm{T}}\mathbf{A}^{-1}\boldsymbol{\Phi}^{\mathrm{T}}\mathbf{y} \\ &= \boldsymbol{\phi}(\boldsymbol{x}_*)^{\mathrm{T}}\Sigma_w\boldsymbol{\Phi}^{\mathrm{T}}\left(\boldsymbol{\Phi}\Sigma_w\boldsymbol{\Phi}^{\mathrm{T}} + \sigma_0^{-2}\mathbf{I}_n\right)^{-1}\mathbf{y}\end{aligned} \tag{1.7}$$

which shows that the new prediction is a weighted average of existing ones in $\boldsymbol{y}$. Here, $\mathbf{I}_n$ is the $n \times n$ identity matrix. The variance of the prediction is

$$\begin{aligned}\mathbb{V}[Y(\boldsymbol{x}_*)] &= \boldsymbol{\phi}(\boldsymbol{x}_*)^{\mathrm{T}}\mathbf{A}^{-1}\boldsymbol{\phi}(\boldsymbol{x}_*) + \sigma_0^2 \\ &= \boldsymbol{\phi}(\boldsymbol{x}_*)^{\mathrm{T}}\left(\boldsymbol{\Sigma}_w - \boldsymbol{\Sigma}_w\boldsymbol{\Phi}^{\mathrm{T}}\left(\boldsymbol{\Phi}\boldsymbol{\Sigma}_w\boldsymbol{\Phi}^{\mathrm{T}} + \sigma_0^2\mathbf{I}_n\right)^{-1}\boldsymbol{\Phi}\boldsymbol{\Sigma}_w\right)\boldsymbol{\phi}(\boldsymbol{x}_*) + \sigma_0^2\end{aligned} \tag{1.8}$$

It is important to note the difference in computational complexity of the two above equivalent ways presented in the foregoing to calculate the mean and variance of prediction. The computational bottleneck involves the inversion of covariance matrices. The size of matrix $\mathbf{A}$ is $m \times m$, whereas the size of $\left(\boldsymbol{\Phi}\boldsymbol{\Sigma}_w\boldsymbol{\Phi}^{\mathrm{T}} + \sigma_0^2\mathbf{I}_n\right)$ is $n \times n$. Therefore, the complexities of computation increase in the orders of $O\left(m^3\right)$ and $O\left(n^3\right)$, respectively.

Gaussian process regression can be applied to construct the surrogates for simulations where the closed-form input−output functional relationships are not available. That is, Eq. (1.2) serves as the surrogate with input $\boldsymbol{x}$ and output Y. Based on the simulation data, hyperparameters $\boldsymbol{w}$ can be trained and obtained from Eq. (1.6). The predictions of means and variances for a new input are calculated based on Eqs. (1.7) and (1.8), respectively. More complex kernel functions with more hyperparameters can also be introduced. The training of hyperparameters can be done by maximizing the likelihood, similar to Eq. (1.5).

The major challenge of using Gaussian process regression is the computational complexity for high-dimensional problems. As the dimension of input $\boldsymbol{x}$ increases, the required number of training samples n grows exponentially in order to have a good coverage of the high-dimensional input space. Major research efforts have been given to improve the computational efficiency with large datasets. Besides traditional data processing techniques for dimension reduction (e.g., principal component analysis, factor analysis, and manifold learning), integrated statistical and computational methods have been developed. The first approach is to reduce the rank of the covariance matrix. For instance, a selected subset of samples can be taken to construct

a sub-Gaussian process to predict the original process [38,39]. In fixed ranking kriging, the covariance matrix is projected into a fixed dimensional space so that the inversion relies on the fixed-rank matrix in the projected space [40]. Based on the Karhunen–Loéve expansion to approximate the covariance function, the inverse of the covariance matrix can be obtained with reduced-rank approximation [41,42]. Gaussian Markov random field on sparse grid has also been used to approximate covariance [42]. The second approach is to reduce the computational complexity with the sparse approximation of covariance matrices. For instance, the spatial localization of covariance functions leads to sparse (or tapered) covariance matrices, and the inverse of sparse matrices can be computed more efficiently [43,44]. The bias introduced by the tapering also needs to be compensated [45]. Sequential sampling or active learning can also be applied to update the subset of data in approximation of the global model [46]. The third approach is using sparse spectral approximation of covariance functions, where a finite set of basis functions are chosen in the construction. For instance, sinusoidal functions [47,48] have been applied in the spectral approximation. The fourth approach to deal with the large dataset is distributed or clustered kriging, where the data are subdivided into subsets and multiple surrogate models are constructed. The new value is predicted as the weighted average of predictions from multiple models. The weights can be determined by an optimization procedure to minimize the predicted variance [49], the distances between the input to predict and the centers of clusters [50], or the Wasserstein distances between the Gaussian posteriors of the main cluster and the neighboring ones [51].

One issue with universal kriging for UQ is that the mean response is usually assumed to follow the polynomial form. Therefore, model form uncertainty is introduced in terms of particular orders of polynomial basis functions. To improve the accuracy of prediction, a Bayesian model update approach with multiple models has been proposed [52]. Similarly, blind kriging modifies polynomials with Bayesian update by incorporating experimental data [53]. As the alternative, sinusoidal functions instead of polynomials have also been used in predicting the mean response [54]. The assumption of covariance functions is another source of model form uncertainty. Stochastic kriging or composite Gaussian process [55,56] methods were introduced to decompose the covariance into two components. One covariance process is from the underlying true function, whereas the other is from experimental data. This approach allows for the decomposition of model form uncertainty. Nevertheless, the assumption of the unknown covariance of the two Gaussian processes still has to be made. One more issue of constructing Gaussian process regression models is the lack of data when extensive simulation runs and/or experiments are costly. Multifidelity cokriging [57,58] is a cost-effective approach for surrogate modeling with the consideration of experimental cost, where low- and high-cost data are combined to construct the surrogate. New sequential sampling strategies can be taken to decide the optimal combination of low- and high-fidelity data [59]. The low- and high-fidelity cokriging model can also be extended to multiple fidelity levels as a recursive model with nested design sites [60].

1.3.5 Bayesian model calibration and validation

One important procedure in modeling and simulation is model calibration, where parameters of physical models need to be tuned to match experimental measurements. Gaussian process regression has been applied in simulation model calibration [61,62]. As an extension of Eq. (1.2), the surrogate for simulations is modeled as a composite Gaussian process in

$$Y(\boldsymbol{x}) = \rho\eta(\boldsymbol{x}, \boldsymbol{\theta}; \boldsymbol{w}) + \delta(\boldsymbol{x}) + \varepsilon \tag{1.9}$$

where $\boldsymbol{\theta}$ are the model parameters to be calibrated, $\eta(\cdot)$ approximates the physical model, and $\delta(\cdot)$ is the model discrepancy. Both $\eta(\cdot)$ and $\delta(\cdot)$ are Gaussian process models. The additional hyperparameter ρ can be introduced as the scaling factor. Combining the simulated dataset $D = \{(\boldsymbol{x}_i, \boldsymbol{\theta}_i, \boldsymbol{y}_i)\}$, where simulations are run with different parameter values $\boldsymbol{\theta}_i$'s and inputs $\boldsymbol{x}_i$'s, with experimental measurements $D' = \{(\boldsymbol{x}_i', y_i')\}$, Eq. (1.9) can be treated as a multivariate Gaussian process regression model with inputs $(\boldsymbol{x}_i, \boldsymbol{\theta}_i)$'s. The model parameters $\boldsymbol{\theta}$ can be similarly trained by maximizing the likelihood, along with all hyperparameters, in the calibration process if the covariance associated with the model parameters is also assumed to be Gaussian. Further extensions of capturing the model discrepancy in the Gaussian processes [63,64] and categorical parameters [65] were also studied.

In a more general setting without the assumption of Gaussian processes, model calibration can be performed by finding parameter values that minimizes the difference between the observation and simulation prediction as the posterior [66,67]. Calibration thus is an optimization process to minimize the difference. Choosing the prior however can affect the accuracy of calibration, especially when there are limited data. Besides parameter calibration, model forms can be calibrated with Bayesian model averaging to incorporate model form errors [68]. Fractional-order derivatives can also be treated as hyperparameters of model forms and similarly calibrated as continuous variables [69].

Model validation is to compare the model predictions with experimental experiments and evaluate the level of agreement [70]. A straightforward comparison is to check the confidence level associated with the difference between the predicted and measured quantities subject to statistical errors [71]. The Bayesian approach for model validation is comparing the prior and posterior probability distributions of the quantities of interests. The prior distribution is from the original model prediction, whereas the posterior is from the prediction after the model parameters are updated with experimental observations. The general criterion is the distance or difference between two probability distributions [72]. The composite Gaussian process model in Eq. (1.9) can also be applied in validation. When the posterior estimation of model bias $\delta(\cdot)$ with consideration of both simulation and experimental data is within an error threshold interval, the model is regarded as valid [73]. Bayesian hypothesis testing can also be applied for validation, where the null and alternative hypotheses are compared after they are updated with experimental observations [74].

1.3.6 Polynomial chaos expansion

Polynomial chaos expansion (PCE) [75–77] approximates random variables in functional or reciprocal space with orthogonal polynomials as bases. In PCE, a stochastic process or random variable is expressed as a spectral expansion in terms of orthogonal eigenfunctions with weights associated with a particular probability density. More specifically, a stochastic process $u(\boldsymbol{x};\boldsymbol{\xi})$ can be approximated as

$$u(\boldsymbol{x};\boldsymbol{\xi}) \approx \sum_{m=1}^{M} \widehat{u}_m(\boldsymbol{x})\Psi_m(\boldsymbol{\xi}) \quad M = \binom{N+P}{N} \tag{1.10}$$

where $\boldsymbol{\xi} = [\xi_1, \ldots, \xi_N]$ is an N-dimensional vector of random variables as parameters of $u(\boldsymbol{x};\boldsymbol{\xi})$ which follows a particular distribution with probability density function $p(\boldsymbol{\xi})$, N-variant P-th order polynomials $\Psi_m(\boldsymbol{\xi})$'s form the orthogonal basis, and $\widehat{u}_m$'s are the PCE coefficients. An example of the expansion is that the Wiener process (also known as Brownian motion) can be written as a spectral expansion in terms of the Hermite polynomials and normal distribution. Different polynomials are available for different probability distributions. For example, Legendre polynomials are for uniform distribution, Jacobi polynomials for beta distribution, Laguerre polynomials for gamma distribution, Charlier polynomials for Poisson, Krawtchouk polynomials for binomial, and Hahn polynomials for hypergeometric. Orthogonality ensures the efficiency of computation and ease of quantifying the truncation error.

The PCE coefficients in Eq. (1.10) can be calculated by projection as

$$\widehat{u}_m(\boldsymbol{x}) = \int u(\boldsymbol{x};\boldsymbol{\xi})\Psi_m(\boldsymbol{\xi})p(\boldsymbol{\xi})\mathrm{d}\boldsymbol{\xi} \tag{1.11}$$

The integral in Eq. (1.11) can be estimated with MC sampling. Yet a much more efficient approach is the quadrature as weighted summation. That is, discrete nodes $\boldsymbol{\xi}^{(k)}$'s and associated weights are predefined, and the integral is calculated as the sum of the weighted values of $u\left(\boldsymbol{x};\boldsymbol{\xi}^{(k)}\right)\Psi_m\left(\boldsymbol{\xi}^{(k)}\right)$. In the nonintrusive PCE, the solution $u\left(\boldsymbol{x};\boldsymbol{\xi}^{(k)}\right)$ with respect to each sample of random variable $\boldsymbol{\xi}^{(k)}$ can be obtained by solving existing the deterministic model or simulation. Because of the orthogonality of polynomial basis, the statistical moments of the random process u can be easily obtained. The mean solution is estimated as

$$\mathbb{E}[u(\boldsymbol{x})] = \int \left(\sum_{m=1}^{M} \widehat{u}_m(\boldsymbol{x})\Psi_m(\boldsymbol{\xi})\right)p(\boldsymbol{\xi})\mathrm{d}\boldsymbol{\xi} = \widehat{u}_1(\boldsymbol{x}) \tag{1.12}$$

The covariance function is

$$\mathbb{C}[u(\boldsymbol{x}_1), u(\boldsymbol{x}_2)] = \sum_{m=2}^{M} \widehat{u}_m(\boldsymbol{x}_1)\widehat{u}_m(\boldsymbol{x}_2) \tag{1.13}$$

The variance function is

$$V[u(\boldsymbol{x})] = \sum_{m=2}^{M} \widehat{u}_m^2(\boldsymbol{x}) \tag{1.14}$$

The nonintrusive PCE approach has been applied to assess the sensitivity of input parameters in reaction−diffusion simulations [78] and perform variance estimation for GSA [79].

Computational efficiency is a challenge for nonintrusive PCE. A large number of samples are required, even though LHS and sparse grid can be applied. Each sample can correspond to a simulation run. Solving a stochastic differential equation is reduced to solving many deterministic differential equations. The efficiency of computation is directly related to the truncation, which also depends on types of distributions and the corresponding polynomials. Some distributions such as those with long and heavy tails cannot be efficiently modeled using PCE approximation.

1.3.7 Stochastic collocation and sparse grid

When the number of input parameters for simulation models is very high, i.e., in the hundreds, the direct construction of the high-dimensional response surface will become inefficient. Stochastic collocation [80,81] is an approach to alleviate the curse of dimensionality. The main idea is to choose the sampling positions of input wisely for functional evaluations in conjunction with the orthogonal polynomials in the problem solving process (i.e., partial differential equation with random inputs) so that a sparse grid [82] can be used. The samples can be selected as the zeros or roots of samples at the sparse grid can be used in either the construction of Lagrange interpolating polynomials or in the pseudospectral with quadrature interpolation.

In the Lagrange interpolation scheme, a set of nodes $\left\{\boldsymbol{\xi}^{(k)}\right\}_{k=1}^{K}$ in the probabilistic parameter space of $u(\boldsymbol{x};\boldsymbol{\xi})$ are predetermined. The solution $u(\boldsymbol{x};\boldsymbol{\xi})$ of a stochastic differential equation can be approximated as

$$u(\boldsymbol{x};\boldsymbol{\xi}) \approx \sum_{k=1}^{K} u\left(\boldsymbol{x};\boldsymbol{\xi}^{(k)}\right) L_k(\boldsymbol{\xi}) \tag{1.15}$$

where $L_k(\cdot)$'s are the Lagrange polynomials, and $u\left(\boldsymbol{x};\boldsymbol{\xi}^{(k)}\right)$ is the solution of the deterministic differential equation when random variable $\boldsymbol{\xi}$ takes the sample value of $\boldsymbol{\xi}^{(k)}$. To obtain $u\left(\boldsymbol{x};\boldsymbol{\xi}^{(k)}\right)$, the existing deterministic solver can be readily applied.

In the pseudospectral interpolation, PCE style expansion is applied instead of the Lagrange interpretation. Similar to Eq. (1.10), the solution is approximated by

$$u(\boldsymbol{x};\boldsymbol{\xi}) \approx \sum_{m=1}^{M} \widehat{c}_m(\boldsymbol{x})\Psi_m(\boldsymbol{\xi}) \quad M = \begin{pmatrix} N+P \\ N \end{pmatrix} \tag{1.16}$$

where the expansion coefficients however are calculated as

$$\widehat{c}_m(\boldsymbol{x}) = \sum_{j=1}^{Q} u\left(\boldsymbol{x};\boldsymbol{\xi}^{(j)}\right)\Psi_m\left(\boldsymbol{\xi}^{(j)}\right)w^{(j)} \tag{1.17}$$

which are the weighted discrete sums realized at the sampled grid locations $\boldsymbol{\xi}^{(j)}$'s. The grid locations $\boldsymbol{\xi}^{(j)}$'s and weights $w^{(j)}$'s are carefully chosen so that the weighted sum can approximate the integral in Eq. (1.11) well.

The grid location selection in stochastic collocation is important for accuracy and efficiency. For a one-dimensional problem, Gauss quadrature is usually the optimal choice. The challenge is high-dimensional cases, where full tensor products will grow the number of grid points exponentially as the dimension increases. Sparse grid method is an approach to cope with the efficiency issue. It was proposed to reduce the number of grid points and improve the efficiency in multidimensional quadrature and interpolation [83] and has been widely applied in stochastic collocation. Instead of full tensor products to generate grids in a high-dimensional sampling space, a much coarser tensorization can be taken in Smolyak's quadrature. The subset of grid points is chosen with recursive hierarchical subspace splitting so that the interpolation can have small approximation errors.

1.3.8 Local sensitivity analysis with perturbation

In contrast to GSA, LSA studies the effect of input uncertainty locally. A straightforward way is to estimate derivatives of models with the finite-difference approach where the difference between two responses is divided by the perturbation of inputs. The finite-difference approach is a nonintrusive approach to assess sensitivity. In addition to these direct (forward) methods, adjoint (backward) SA approaches were also developed for deterministic simulation based on differential equations [84,85]. A more efficient LSA method that is specific for stochastic simulation is to estimate the derivatives of the expected values of output performance, i.e., the expected values of stochastic derivatives or gradients, from simulation directly. This can be achieved by either varying output performance w.r.t. input parameters as the infinitesimal perturbation analysis [86,87] or by varying the probability measures w.r.t. inputs as in the likelihood ratio method [88–90]. These approaches are intrusive in order to promote efficiency of computation.

1.3.9 Polynomial chaos for stochastic Galerkin

Similar to nonintrusive PCE, stochastic Galerkin method relies on polynomial expansion to estimate probability density and propagate parameter uncertainty. The difference is that stochastic Galerkin is an intrusive UQ approach to solve stochastic ordinary or partial differential equations. In the intrusive PCE approach, the target stochastic process $u(\boldsymbol{x};\boldsymbol{\xi})$ is not readily available, and the approach in Eq. (1.11) to calculate PCE coefficients is of no use. Instead, it is assumed that $u(\boldsymbol{x};\boldsymbol{\xi})$ can be

computed based on some physical models (i.e., ordinary and partial differential equations), and the mathematical forms of the models are available. The expansions are substituted for the variables into the differential equations, and the operations on the original variables are applied to the expansions.

1.3.10 Nonprobabilistic approaches

Differing from traditional probabilistic approaches, nonprobabilistic approaches for UQ have been developed. Perhaps the best known is the Dempster–Shafer evidence theory [91,92]. In this theory, evidence is associated with a power set of discrete random events, in contrast to random events in probability theory. Uncertainty is quantified with the so-called basic probability assignment (PBA). As an illustration, if the event space is $\Omega = \{A, B, C\}$, the probability assignments in traditional probability theory are $P(A)$, $P(B)$, and $P(C)$, subject to constraint $P(A) + P(B) + P(C) = 1$. In the Dempster–Shafer theory, imprecision of assignments is allowed. Therefore, probabilistic measures are assigned to the power set of events, $2^{\Omega} = \{\varnothing, \{A\}, \{B\}, \{C\}, \{A, B\}, \{A, C\}, \{B, C\}, \{A, B, C\}\}$. The assignments are BPAs, as $m(\varnothing)$, $m(\{A\})$, …, $m(\{A, B, C\})$, subject to $\sum_{x \in 2^{\Omega}} m(x) = 1$. That is, uncertainty is directly measured with a set of events. As a result, when we try to estimate the uncertainty associated with individual events, the probability becomes not precisely known. Two quantities are associated with each event. One is the lower limit of probability, also known as *belief*, calculated as $\underline{P}(y) = \sum_{x \subseteq y} m(x)$. The other is the upper limit of probability, also known as *plausibility*, calculated as $\overline{P}(y) = \sum_{x \cap y \neq \varnothing} m(x)$. The belief–plausibility pair provides a convenient way to capture epistemic and aleatory uncertainty. The difference between the lower and upper probability limits is epistemic in nature, whereas the probability itself is aleatory.

There are several mathematical formalisms and theories that are very similar to the Dempster–Shafer theory, such as the theory of coherent lower previsions [93], probability box [94], interval probability [95], generalized interval probability [96], etc. These imprecise probability modeling approaches were developed from slightly different perspectives with different interpretations. Another mathematical formalism, random set [97,98], which quantifies uncertainty associated with random sets of events, is also equivalent to the Dempster–Shafer theory and other imprecise probability theories.

In engineering, interval analysis [99–101] has been widely applied to perform sensitivity analysis and model uncertainty propagation. It was originally developed to address the issue of numerical errors in digital computation due to the floating-point representation of numbers. It is based on a generalization in which interval numbers replace real numbers, interval arithmetic replaces real arithmetic, and interval analysis replaces real analysis. In other words, calculation is based on interval numbers with lower and upper limits. Interval provides a distribution-neutral form to represent uncertainty and error in measurement or computation. Similar to confidence interval in

statistics, the bounds provide an estimate of uncertainty, but without the need to keep track of the associated statistical distribution (which typically is computationally expensive to be tracked). Therefore, it is an efficient scheme to quantify uncertainty when statistical information does not need to be kept or is not available due to lack of data.

1.4 UQ in materials modeling

Chernatynskiy et al. [102] and Wang [103] previously provided reviews on UQ in multiscale materials simulation. This section focuses on an overview of research efforts in the most recent years of rapid growth of interest in UQ for ICME.

1.4.1 UQ for ab initio and DFT calculations

Model form error in first principles simulation has been recently explored. Formal UQ methods have been applied to quantify uncertainty in DFT calculations. Particularly, Bayesian approach to estimate the errors associated with DFT exchange-correlation functionals by incorporating experimental data has been extensively studied, including GGA [104], van der Waals interactions [105], meta-GGA [106,107], and Bayesian model calibration [108]. Regression analysis has also been used to predict the systematic errors associated with the exchange-correlation functionals for different crystal structures [109,110]. Gaussian process regression has been applied to construct surrogates of potential energy surface and quantify errors from DFT calculations [50,111−113]. Generalized polynomial chaos was also applied to construct surrogate of energy surface [114]. Other UQ methods such as LSA [115] and resampling [116] are used to estimate the error distribution of DFT calculations.

In addition to UQ methods, comprehensive comparisons of accuracy among ab initio methods have been studied. Irikura et al. [117] studied the bias in vibration frequency predictions of Hartree-Fock with 40 different basis sets. Lejaeghere et al. [118,119] provided a comprehensive quantitative error analysis for DFT energy predictions from over 40 different methods including all-electron, projector-augmented wave (PAW), ultrasoft (USPP), and norm-conserving pseudopotential (NCPP). It is seen that model form errors increase because of simplification and approximation in order to gain computational time. Tran et al. [120] compared the error of Rungs 1 to 4 in DFT Jacob's ladder based on lattice constant, bulk modulus, and cohesive energy of solids.

1.4.2 UQ for MD simulation

Uncertainty in materials simulation was first recognized with sensitivity of interatomic potential selection in MD simulation of solid materials [121,122], water molecule [123,124], irradiation damage [125], and others, as well as the effect of cut-off radius. Only recently, formal UQ methods have been applied.

To construct better interatomic potentials in MD, Bayesian calibration has been extensively applied to different potentials such as MEAM [126], Lennard-Jones [127−129], TIP4P [130,131], and coarse-grained MD models [132,133]. Based on experimental observations, the parameters of potentials are adjusted to maximize the likelihood. The major challenge of Bayesian approach is the computational load of Markov chain Monte Carlo involved in estimating the posterior. Numerical approximations can be applied to improve the efficiency [134,135].

Surrogate modeling can also be applied to construct response surfaces from MD simulations as the structure−property relationships to predict material properties. The uncertainty associated with property predictions with respect to interatomic potential parameters can also be evaluated based on surrogate modeling. The modeling methods such as PCE [136,137], Kriging [138], and Lagrange interpolation [139] have been used to assess the uncertainty effect or sensitivity of interatomic potentials on MD simulations.

Instead of constructing response surfaces, the straightforward sensitivity analysis can be done by varying the values of input parameter values based on factorial experimental design [140,141] or MC sampling [142−144]. The above UQ and sensitivity analysis approaches are categorized as nonintrusive, where MD simulation is treated as a black box. Data are collected as input−output pairs for response analysis. Therefore, multiple runs of simulations are needed. Different from the above, Tran and Wang [145,146] developed an interval-based MD mechanism via Kaucher interval arithmetic to assess sensitivities on-the-fly. This is an intrusive approach where the detailed knowledge of MD simulation is needed and simulation packages need to be modified. The new MD simulation tool is an extension [147] of original LAMMPS [148]. Only one run of MD simulation is enough to predict the propagation of uncertainty. Also as gray-box approaches, Tsourtis et al. [149] measured the state distribution variation with respect to the model parameter perturbation in the Langevin dynamics of MD, where only two simulation runs are needed for sensitivity analysis. Reeve and Strachan [150] developed a functional local perturbation approach based on the knowledge of interatomic potential forms to estimate computational prediction errors associated with the Lennard-Jones potential.

Sensitivity analyses exploring uncertainty of MD simulations have gone beyond consideration of interatomic potentials. For instance, Patrone et al. [151] evaluated the variabilities of model size and simulation time on the glass transition temperature of polymers. Kim et al. [152] studied the effects of model size and simulation time on the shear viscosity prediction by the Green−Kubo formulation. Alzate-Vargas et al. [153] assessed the sensitivities of molecular weight, force field, and data analysis scheme in predicting glass transition of polymers.

1.4.3 UQ for meso- and macroscale materials modeling

UQ methods have been widely applied at macroscale or continuum level modeling and simulation. Particularly related to structural materials, methods of Karhunen−Loève expansion [154], PCE [155], and Kriging [156] for Gaussian and non-Gaussian processes or random fields have been well studied in stochastic mechanics given the

variability of material distributions [157,158]. Multiphase material morphology and corresponding properties have been modeled by non-Gaussian random fields such as level-cut filtered Poisson field [159], Markov random field [160], and nonparametric random field [161]. Porosity in solid structures can also be modeled by Gaussian random fields and integrated in FEA [162]. In addition to Karhunen–Loève and polynomial expansions, random fields can also be approximated by Fourier series [163], autoregressive moving average [164], and wavelets [165].

Because of missing physics in traditional ordinary and partial differential equations, stochastic versions of ordinary and partial differential equations have been introduced, where loads or coefficients are random variables, to capture the randomness of material properties and behaviors. Stochastic partial differential equations can be solved by MC sampling, or more efficiently by second-order moment approximation [166], Neumann expansion [167], interval convex method [168,169], Karhunen–Loève expansion [170], stochastic collocation [80,171–173], and PCE [64,77,174]. For stochastic differential equations, Fokker–Planck equation [175] that is equivalent to the Itô process can be formulated to simulate evaluation of probability distributions in dynamics simulation such as Langevin dynamics. Real physical processes, however, are not perfectly Markovian although they may be Gaussian. Generalization of the Fokker–Planck equation thus is needed. For example, generalized Fokker–Planck equation with time-dependent friction coefficients can model the velocity field of Brownian particles subjected to arbitrary stochastic forces [176]. A generalization with a memory kernel introduced in the diffusion coefficient simulates the Brownian motion of particles in viscoelastic fluid more accurately [177]. Non-Gaussian Brownian and Lévy processes can be modeled through transformations or mappings to Gaussian–Markovian process [178].

Traditional models of random fields as well as statics and dynamics behaviors cannot efficiently capture the physical complexity of material properties such as memory effects and energy dissipation in viscoelastic materials, fractal porous media, liquid–solid mixture, sub- and superdiffusive transport, etc. Fractional calculus has been introduced to reduce the model form error caused by traditional integer-order integrals and derivatives [69]. For instance, the viscoelastic behavior of materials is modeled more efficiently with fractional derivatives [179]. The sub- and superdiffusion can be captured by the fractional Langevin equation [180]. The effective reaction–diffusion process in porous media can be modeled as Lévy process [181]. Fractional-order continuum mechanics for fractal solid materials was also introduced [182].

UQ for mesoscale simulations is relatively unexplored. For instance, in PF simulation of solidification, the majority of existing work remained on sensitivity analysis on the model parameters, such as solute expansion factor [183], convection [184], grain orientation [185], and latent heat [186]. Recently, the nonintrusive PCE was applied to quantify the effects of microstructural parameters and material properties on the macrosegregation and solidification time [187] and microstructure [188] in PF simulations. To alleviate the numerical instability in simulation because of model approximation, empirical antitrapping current term can be introduced [189]. Stochastic Cahn–Hilliard equation [190] and stochastic Allen–Cahn equation [191] have been studied.

Fractional Cahn−Hilliard and Allen−Cahn equations [192] were also introduced to mitigate model form uncertainty.

1.4.4 UQ for multiscale modeling

One unique need of UQ for materials modeling is the multiscale nature of simulation predictions. Model calibration and validation may have to be based on experimental observations of QoIs that are different from the predicted QoIs at a different length or time scale. To enable cross-scale or cross-domain information fusion, Bayesian approaches based on different information sources in sensing and modeling can be done, where the hidden or latent variables can be introduced as in hidden Markov models [193], and cross-scale model calibration and validation with epistemic and aleatory uncertainties can be accomplished [194,195]. The hidden Markov model can also be used to establish the connection between coarse-grain and fine-grain model parameters [196]. Even at the same scale, different models may exist to describe the same QoIs. Bayesian approaches can also be taken to reconcile model inconsistency. For example, to calibrate crystal plasticity models and combine models derived from bottom-up atomistic simulations and top-down experimental measurements, the maximum likelihood criterion can be extended to include the constraints of model parameter inconsistency [197] or model form discrepancy [198] so that the regularized likelihood incorporates different sources of information. The Bayesian model average approach can also be taken to reconcile the discrepancy between predictions of QoIs from different scales, e.g., between quantum and molecular level simulations [199].

Another unique need of UQ for materials modeling is to support cross-scale uncertainty propagation. QoIs predicted by simulations at different scales are usually coupled, as the outputs of a smaller-scale simulation can be the required inputs for a larger-scale simulation. To model cross-scale uncertainty propagation, Bostanabad et al. [200] developed a nested random field approach where the hyperparameters of an ensemble of random fields at the lower scale is characterized by yet another random field at the upper scale. Variations and perturbations can be applied in the input−output relationships between different simulation models, such as from MD to PF, DD, and crystal elasticity, to assess the sensitivities [201].

1.4.5 UQ in materials design

Design is an iterative process of searching feasible solutions and identifying in some sense the optimal subset during which decisions are made based on available information. Uncertainty needs to be incorporated in engineering and materials design for robustness consideration. UQ methods have been applied for robust design of structural materials given the uncontrollable factors in complex fabrication processes. For instance, polynomial regressions have been used as surrogates for simulations in simulation-based robust design of materials [202]. The constructed response surface models as the structure−property relationships can be applied to identify feasible design space and search for the optimum [203]. In junction with atomistic simulations, nanoscale materials can also be designed with the optimum macroscopic properties,

for instance, the maximum yield strength of nanowires under the uncertainty associated with environment variables (e.g., strain rate, temperature, and size) [204]. When multiple design objectives are considered, the Pareto frontier can also be identified efficiently aided by the response surfaces [205]. Most recently, Bayesian optimization is recognized as a useful tool for robust global optimization. Instead of the original design objective, an acquisition function is used as the utility function to guide the sequential sampling process to construct Gaussian process surrogates [51,206]. The uncertainty associated with simulation predictions thus can be considered, and a balance between exploration and exploitation is achieved. Acquisition functions such as the expected improvement function can be used in designing NiTi-based alloys with the minimum thermal dissipation based on Bayesian optimization [205,207].

To quantify the uncertainty in materials, random fields have a unique advantage of modeling spatial distributions of phases or properties. Random fields have been used to predict the stochasticity of material properties as well as uncertainty propagation between design parameters so that the response surfaces at multiple scales can be constructed applied for multilevel robust optimization [208]. For topological optimization of materials and metamaterials, the robustness of optimal topology can be improved by incorporating random fields of loads [209,210]. The random material distributions can also be modeled with polynomial chaos [211]. For robust topological optimization, local sensitivities of geometry and topology variations [212,213], manufacturing errors [214], and external loads [215,216] with respect to the optimal solutions need to be assessed. The simultaneous considerations of mean and variance in design objectives with confidence bounds are typically needed to ensure robustness [217].

1.5 Concluding remarks

Uncertainty is an inherent factor in various aspects of modeling, design, and development of materials. Aleatory uncertainty or randomness has been a core focus in physics, e.g., quantum mechanics and statistical mechanics. Nevertheless, the importance of epistemic uncertainty was only recognized more recently in the research community of materials science and engineering. Given the limitations of both experimental observation and physics-based modeling, the lack of knowledge is the most common cause of uncertainty in materials. This is manifested primarily as approximation and simplification. Compared to most science and engineering disciplines, materials research faces specific challenges in bridging the knowledge gap from the scale of electrons and atoms in physics to the scale of homogenized material properties that support traditional engineering design. Uncertainty naturally arises from the lack of good physical models to address phenomena at different length and time scales, as well as the lack of data for calibration and validation of complex empirical or semiempirical models. Obviously elevating the level of knowledge is the ultimate solution to reduce epistemic uncertainty. This will lead to higher quality and more powerful physical models in the future. Along the way, acknowledging the uncertainty and imperfection associated

with existing models is essential to advance scientific discovery and exploit the control of structure to enable materials design and development.

Developing practical UQ tools for the materials domain that are scalable for high-dimensional complex problems is also essential. Most of existing tools can be mathematically sound for small and academic problems. However, they are often not applicable to ICME because of its special needs, including high-dimensionality of the design space, operation of phenomena at multiple length and time scales, both short- and long-range phenomena of interest, and parallel and high-performance computing environments. Development of domain-oriented UQ methods for these particular needs is relevant to this community.

Acknowledgments

This work was supported in part by the National Science Foundation under grants CMMI-1306996, CMMI 1761553, and the US Department of Energy Office of Nuclear Energy's Nuclear Energy University Programs.

References

[1] P.M. Pollock, J.E. Allison, Integrated computational materials engineering: a transformational discipline for improved competitiveness and national security, in: Committee on Integrated Computational Materials Engineering, National Materials Advisory Board, Division of Engineering and Physical Sciences, National Research Council of the National Academies, National Academies Press, Washington, DC, 2008.

[2] D.L. McDowell, D. Backman, Simulation-assisted design and accelerated insertion of materials, in: S. Ghosh, D. Dimiduk (Eds.), Computational Methods for Microstructure-Property Relationships, Springer, 2011, ISBN 978-1-4419-0642-7, pp. 617−647. Ch. 19.

[3] J.P. Holdren, National Science and Technology Council, Committee on Technology, Subcommittee on the Materials Genome Initiative, Materials Genome Initiative Strategic Plan, 2014. https://www.nist.gov/sites/default/files/documents/2018/06/26/mgi_strategic_plan_-_dec_2014.pdf.

[4] C. Featherston, E. O'Sullivan, A Review of International Public Sector Strategies and Roadmaps: A Case Study in Advanced Materials, Centre for Science Technology and Innovation, Institute for Manufacturing. University of Cambridge, UK, 2014. https://www.ifm.eng.cam.ac.uk/uploads/Resources/Featherston__OSullivan_2014_-_A_review_of_international_public_sector_roadmaps-_advanced_materials_full_report.pdf.

[5] D.L. McDowell, Microstructure-sensitive computational structure-property relations in materials design, in: D. Shin, J. Saal (Eds.), Computational Materials System Design, Springer, Cham, 2018, pp. 1−25.

[6] G.B. Olson, Genomic materials design: the ferrous frontier, Acta Mater. 61 (3) (2013) 771−781.

[7] Y. Wang, L. Swiler, Special issue on uncertainty quantification in multiscale system design and simulation, ASCE-ASME J. Risk Uncertain. Eng. Syst. Part B Mech. Eng. 4 (1) (2018) 010301.

[8] D.L. McDowell, Multiscale modeling of interfaces, dislocations, and dislocation field plasticity, in: S. Mesarovic, S. Forest, H. Zbib (Eds.), Mesoscale Models: From Microphysics to Macro-Interpretation, Springer, 2019, pp. 195−297.
[9] J.C. Helton, J.D. Johnson, W.L. Oberkampf, An exploration of alternative approaches to the representation of uncertainty in model predictions, Reliab. Eng. Syst. Saf. 85 (1) (2004) 39−71.
[10] D.E. Lehmer, Mathematical methods in large-scale computing units, in: Proc. 2nd Symp. On Large-Scale Digital Calculating Machinery, Harvard University Press, Cambridge, MA, 1951, pp. 141−146.
[11] A. Rotenberg, A new pseudo-random number generator, J. Assoc. Comput. Mach. 7 (1) (1960) 75−77.
[12] T.E. Hull, A.R. Dobell, Random number generators, SIAM Rev. 4 (3) (1962) 230−254.
[13] L. Kuipers, H. Niederreiter, Uniform Distribution of Sequences, Interscience, New York, 1974.
[14] J.E. Gentle, Random Number Generation and Monte Carlo Methods, second ed., Springer, New York, 2003.
[15] J. Eichenauer, J. Lehn, A non-linear congruential pseudo random number generator, Stat. Hefte (Neue Folge) 27 (1) (1986) 315−326.
[16] P. L'ecuyer, Efficient and portable combined random number generators, Commun. ACM 31 (6) (1988) 742−751.
[17] R.C. Tausworthe, Random numbers generated by linear recurrence modulo two, Math. Comput. 19 (90) (1965) 201−209.
[18] T.G. Lewis, W.H. Payne, Generalized feedback shift register pseudorandom number algorithm, J. Assoc. Comput. Mach. 20 (3) (1973) 456−468.
[19] M. Matsumoto, T. Nishimura, Mersenne twister: a 623-dimensionally equidistributed uniform pseudo-random number generator, ACM Trans. Model Comput. Simulat 8 (1) (1998) 3−30.
[20] D.E. Burmaster, A.M. Wilson, An introduction to second-order random variables in human health risk assessments, Hum. Ecol. Risk Assess. Int. J. 2 (4) (1996) 892−919.
[21] S. Ferson, What Monte Carlo methods cannot do, Human and Ecological Risk Assessment 2 (4) (1996) 990−1007.
[22] A. Saltelli, M. Ratto, T. Andres, F. Campolongo, J. Cariboni, D. Gatelli, M. Saisana, S. Tarantola, Global Sensitivity Analysis: The Primer, John Wiley & Sons, Chichester, West Sussex, England, 2008.
[23] I.M. Sobol', Global sensitivity indices for nonlinear mathematical models and their Monte Carlo estimates, Math. Comput. Simulat. 55 (1) (2001) 271−280.
[24] R.L. Iman, S.C. Hora, A robust measure of uncertainty importance for use in fault tree system analysis, Risk Anal. 10 (3) (1990) 401−406.
[25] T. Homma, A. Saltelli, Importance measures in global sensitivity analysis of nonlinear models, Reliab. Eng. Syst. Saf. 52 (1) (1996) 1−17.
[26] M.H. Chun, S.J. Han, N.I. Tak, An uncertainty importance measure using a distance metric for the change in a cumulative distribution function, Reliab. Eng. Syst. Saf. 70 (3) (2000) 313−321.
[27] E. Borgonovo, A new uncertainty importance measure, Reliab. Eng. Syst. Saf. 92 (6) (2007) 771−784.
[28] J. Hu, Y. Wang, A. Cheng, Z. Zhong, Sensitivity analysis in quantified interval constraint satisfaction problems, J. Mech. Des. 137 (4) (2015) 041701.
[29] G.E. Box, N.R. Draper, Empirical Model-Building and Response Surfaces, Wiley, New York, 1987.

[30] J.P. Kleijnen, Statistical Tools for Simulation Practitioners, Marcel Dekker, 1986.
[31] R.H. Myers, D.C. Montgomery, C.M. Anderson-Cook, Response Surface Methodology: Process and Product Optimization Using Designed Experiments, John Wiley & Sons, 2009.
[32] M.D. McKay, R.J. Beckman, W.J. Conover, Comparison of three methods for selecting values of input variables in the analysis of output from a computer code, Technometrics 21 (2) (1979) 239−245.
[33] R.L. Iman, J.M. Davenport, D.K. Ziegler, Latin Hypercube Sampling (Program User's Guide), Sandia National Laboratories, Albuquerque, NM, 1980. Technical Report SAND79-1473.
[34] J.C. Helton, F.J. Davis, Latin hypercube sampling and the propagation of uncertainty in analyses of complex systems, Reliab. Eng. Syst. Saf. 81 (1) (2003) 23−69.
[35] R.L. Iman, W.J. Conover, Small sample sensitivity analysis techniques for computer models with an application to risk assessment, Commun. Stat. Theor. Methods 9 (17) (1980) 1749−1842.
[36] G. Matheron, Principles of geostatistics, Econ. Geol. 58 (8) (1963) 1246−1266.
[37] N. Cressie, The origins of kriging, Math. Geol. 22 (3) (1990) 239−252.
[38] S. Banerjee, A.E. Gelfand, A.O. Finley, H. Sang, Gaussian predictive process models for large spatial data sets, J. R. Stat. Soc. Ser. B 70 (4) (2008) 825−848.
[39] A.O. Finley, H. Sang, S. Banerjee, A.E. Gelfand, Improving the performance of predictive process modeling for large datasets, Comput. Stat. Data Anal. 53 (8) (2009) 2873−2884.
[40] N. Cressie, G. Johannesson, Fixed rank kriging for very large spatial data sets, J. R. Stat. Soc. Ser. B 70 (1) (2008) 209−226.
[41] H. Sang, J.Z. Huang, A full scale approximation of covariance functions for large spatial data sets, J. R. Stat. Soc. Ser. B 74 (1) (2012) 111−132.
[42] L. Hartman, O. Hössjer, Fast kriging of large data sets with Gaussian Markov random fields, Comput. Stat. Data Anal. 52 (5) (2008) 2331−2349.
[43] R. Furrer, M.G. Genton, D. Nychka, Covariance tapering for interpolation of large spatial datasets, J. Comput. Graph. Stat. 15 (3) (2006) 502−523.
[44] S. Sakata, F. Ashida, M. Zako, An efficient algorithm for Kriging approximation and optimization with large-scale sampling data, Comput. Methods Appl. Mech. Eng. 193 (3−5) (2004) 385−404.
[45] C.G. Kaufman, M.J. Schervish, D.W. Nychka, Covariance tapering for likelihood-based estimation in large spatial data sets, J. Am. Stat. Assoc. 103 (484) (2008) 1545−1555.
[46] R.B. Gramacy, D.W. Apley, Local Gaussian process approximation for large computer experiments, J. Comput. Graph. Stat. 24 (2) (2015) 561−578.
[47] M. Lázaro-Gredilla, J. Quiñonero-Candela, C.E. Rasmussen, A.R. Figueiras-Vidal, Sparse spectrum Gaussian process regression, J. Mach. Learn. Res. 11 (2010) 1865−1881.
[48] A. Gijsberts, G. Metta, Real-time model learning using incremental sparse spectrum Gaussian process regression, Neural Netw. 41 (2013) 59−69.
[49] B. van Stein, H. Wang, W. Kowalczyk, T. Bäck, M. Emmerich, Optimally weighted cluster kriging for big data regression, in: Proc. International Symposium on Intelligent Data Analysis, IDA 2015, October 2015, pp. 310−321.
[50] A. Tran, L. He, Y. Wang, An efficient first principles saddle point searching method based on distributed kriging metamodels, ASCE-ASME Journal of Risk and Uncertainty in Engineering Systems, Part B 4 (1) (2018) 011006.

[51] A.V. Tran, M.N. Tran, Y. Wang, Constrained mixed integer Gaussian mixture Bayesian optimization and its applications in designing fractal and auxetic metamaterials, Struct. Multidiscip. Optim. 59 (6) (2019) 2131−2154.
[52] M.C. Kennedy, A. O'Hagan, Predicting the output from a complex computer code when fast approximations are available, Biometrika 87 (1) (2000) 1−13.
[53] V.R. Joseph, Y. Hung, A. Sudjianto, Blind kriging: a new method for developing metamodels, J. Mech. Des. 130 (3) (2008) 031102.
[54] L.S. Tan, V.M. Ong, D.J. Nott, A. Jasra, Variational inference for sparse spectrum Gaussian process regression, Stat. Comput. 26 (6) (2016) 1243−1261.
[55] B. Ankenman, B.L. Nelson, J. Staum, Stochastic kriging for simulation metamodeling, Oper. Res. 58 (2) (2010) 371−382.
[56] S. Ba, V.R. Joseph, Composite Gaussian process models for emulating expensive functions, Ann. Appl. Stat. 6 (4) (2012) 1838−1860.
[57] A.I. Forrester, A. Sóbester, A.J. Keane, Multi-fidelity optimization via surrogate modelling, in: Proceedings of the Royal Society of London A: Mathematical, Physical and Engineering Sciences, vol. 463, December 2007, pp. 3251−3269. No. 2088.
[58] Z.H. Han, S. Görtz, Hierarchical kriging model for variable-fidelity surrogate modeling, AIAA J. 50 (9) (2012) 1885−1896.
[59] Q. Zhou, Y. Wang, S.K. Choi, P. Jiang, X. Shao, J. Hu, A sequential multi-fidelity metamodeling approach for data regression, Knowl. Based Syst. 134 (2017) 199−212.
[60] L. Le Gratiet, J. Garnier, Recursive co-kriging model for design of computer experiments with multiple levels of fidelity, Int. J. Uncertain. Quantification 4 (5) (2014) 365−386.
[61] M.C. Kennedy, A. O'Hagan, Bayesian calibration of computer models, J. R. Stat. Soc. Ser. B 63 (3) (2001) 425−464.
[62] D. Higdon, J. Gattiker, B. Williams, M. Rightley, Computer model calibration using high-dimensional output, J. Am. Stat. Assoc. 103 (482) (2008) 570−583.
[63] V.R. Joseph, H. Yan, Engineering-driven statistical adjustment and calibration, Technometrics 57 (2) (2015) 257−267.
[64] Y. Ling, J. Mullins, S. Mahadevan, Selection of model discrepancy priors in Bayesian calibration, J. Comput. Phys. 276 (2014) 665−680.
[65] C.B. Storlie, W.A. Lane, E.M. Ryan, J.R. Gattiker, D.M. Higdon, Calibration of computational models with categorical parameters and correlated outputs via Bayesian smoothing spline ANOVA, J. Am. Stat. Assoc. 110 (509) (2015) 68−82.
[66] R. Tuo, C.J. Wu, Efficient calibration for imperfect computer models, Ann. Stat. 43 (6) (2015) 2331−2352.
[67] M. Plumlee, Bayesian calibration of inexact computer models, J. Am. Stat. Assoc. 112 (519) (2017) 1274−1285.
[68] J.A. Hoeting, D. Madigan, A.E. Raftery, C.T. Volinsky, Bayesian model averaging: a tutorial, Stat. Sci. 14 (4) (1999) 382−401.
[69] Y. Wang, Model-form calibration in drift-diffusion simulation using fractional derivatives, ASCE-ASME J. Risk Uncertainty Eng. Syst. Part B 2 (3) (2016) 031006.
[70] W.L. Oberkampf, T.G. Trucano, C. Hirsch, Verification, validation, and predictive capability in computational engineering and physics, Appl. Mech. Rev. 57 (5) (2004) 345−384.
[71] W.L. Oberkampf, M.F. Barone, Measures of agreement between computation and experiment: validation metrics, J. Comput. Phys. 217 (1) (2006) 5−36.
[72] I. Babuška, F. Nobile, R. Tempone, A systematic approach to model validation based on Bayesian updates and prediction related rejection criteria, Comput. Methods Appl. Mech. Eng. 197 (29−32) (2008) 2517−2539.

[73] S. Wang, W. Chen, K.L. Tsui, Bayesian validation of computer models, Technometrics 51 (4) (2009) 439−451.
[74] Y. Ling, S. Mahadevan, Quantitative model validation techniques: new insights, Reliab. Eng. Syst. Saf. 111 (2013) 217−231.
[75] R. Ghanem, P.D. Spanos, Polynomial chaos in stochastic finite elements, J. Appl. Mech. 57 (1) (1990) 197−202.
[76] D. Xiu, G.E. Karniadakis, The Wiener–Askey polynomial chaos for stochastic differential equations, SIAM J. Sci. Comput. 24 (2) (2002) 619−644.
[77] B.J. Debusschere, H.N. Najm, P.P. Pébay, O.M. Knio, R.G. Ghanem, O.P. Le Maître, Numerical challenges in the use of polynomial chaos representations for stochastic processes, SIAM J. Sci. Comput. 26 (2) (2004) 698−719.
[78] M.T. Reagana, H.N. Najm, R.G. Ghanem, O.M. Knio, Uncertainty quantification in reacting-flow simulations through non-intrusive spectral projection, Combust. Flame 132 (3) (2003) 545−555.
[79] B. Sudret, Global sensitivity analysis using polynomial chaos expansions, Reliab. Eng. Syst. Saf. 93 (7) (2008) 964−979.
[80] I. Babuška, F. Nobile, R. Tempone, A stochastic collocation method for elliptic partial differential equations with random input data, SIAM J. Numer. Anal. 45 (3) (2007) 1005−1034.
[81] M.S. Eldred, Recent advances in non-intrusive polynomial chaos and stochastic collocation methods for uncertainty analysis and design, in: Proc. 50th AIAA/ASME/ASCE/AHS/ASC Structures, Structural Dynamics, and Materials Conference, May 4-7, 2009, Palm Springs, California AIAA Paper#2009-2274, 2009.
[82] T. Gerstner, M. Griebel, Numerical integration using sparse grids, Numer. Algorithms 18 (3−4) (1998) 209.
[83] S.A. Smolyak, Quadrature and interpolation formulas for tensor products of certain classes of functions, Dokl. Akad. Nauk. 148 (No. 5) (1963) 1042−1045 (Russian Academy of Sciences).
[84] D.G. Cacuci, Sensitivity theory for nonlinear systems. I. Nonlinear functional analysis approach, J. Math. Phys. 22 (12) (1981) 2794−2802.
[85] G.Z. Yang, N. Zabaras, An adjoint method for the inverse design of solidification processes with natural convection, Int. J. Numer. Methods Eng. 42 (6) (1998) 1121−1144.
[86] Y.C. Ho, X.-R. Cao, Optimization and perturbation analysis of queueing networks, J. Optim. Theory Appl. 40 (1983) 559−582.
[87] R. Suri, M. Zazanis, Perturbation analysis gives strongly consistent estimates for the M/G/1 queue, Manag. Sci. 34 (1988) 39−64.
[88] M.I. Reiman, A. Weiss, Sensitivity analysis via likelihood ratio, in: Proc. Of the 1986 Winter Simulation Conference, 1986, pp. 285−289.
[89] P. Glynn, Likelihood ratio gradient estimation for stochastic systems, Commun. ACM 33 (1990) 75−84.
[90] R.Y. Rubinstein, A. Shapiro, Discrete Event Systems: Sensitivity Analysis and Stochastic Optimization via the Score Function Method, John Wiley & Sons, 1993.
[91] A.P. Dempster, Upper and lower probabilities induced by a multivalued mapping, Ann. Math. Stat. 38 (2) (1967) 325−339.
[92] G. Shafer, A Mathematical Theory of Evidence, Princeton University Press, Princeton, N.J, 1976.
[93] P. Walley, Statistical Reasoning with Imprecise Probabilities, Chapman and Hall, London, 1991.

[94] S. Ferson, V. Kreinovick, L. Ginzburg, D.S. Myers, F. Sentz, Constructing Probability Boxes and Dempster-Shafer Structures, Sandia National Laboratories, 2003. SAND2002-4015.
[95] K. Weichselberger, The theory of interval-probability as a unifying concept for uncertainty, Int. J. Approx. Reason. 24 (2−3) (2000) 149−170.
[96] Y. Wang, Imprecise probabilities based on generalized intervals for system reliability assessment, Int. J. Reliab. Saf. 4 (4) (2010) 319−342.
[97] I.S. Molchanov, Theory of Random Sets, Springer, London, 2005.
[98] H.T. Nguyen, An Introduction to Random Sets, Chapman and Hall/CRC, Boca Raton, 2006.
[99] R.E. Moore, Interval Analysis, Prentice-Hall, Englewood Cliffs, N.J, 1966.
[100] L. Jaulin, M. Kieffer, O. Didrit, E. Walter, Applied Interval Analysis: With Examples in Parameter and State Estimation, in: Robust Control and Robotics, vol. 1, Springer Science & Business Media, 2001.
[101] R.E. Moore, R.B. Kearfott, M.J. Cloud, Introduction to Interval Analysis, vol. 110, SIAM, 2009.
[102] A. Chernatynskiy, S.R. Phillpot, R. LeSar, Uncertainty quantification in multiscale simulation of materials: a prospective, Annu. Rev. Mater. Res. 43 (2013) 157−182.
[103] Y. Wang, Uncertainty in materials modeling, simulation, and development for ICME, in: Proc. 2015 Materials Science and Technology, 2015.
[104] J.J. Mortensen, K. Kaasbjerg, S.L. Frederiksen, J.K. Nørskov, J.P. Sethna, K.W. Jacobsen, Bayesian error estimation in density-functional theory, Phys. Rev. Lett. 95 (21) (2005) 216401.
[105] J. Wellendorff, K.T. Lundgaard, A. Møgelhøj, V. Petzold, D.D. Landis, J.K. Nørskov, T. Bligaard, K.W. Jacobsen, Density functionals for surface science: exchange-correlation model development with Bayesian error estimation, Phys. Rev. B 85 (2012) 235149.
[106] J. Wellendorff, K.T. Lundgaard, K.W. Jacobsen, T. Bligaard, mBEEF: an accurate semi-local Bayesian error estimation density functional, J. Chem. Phys. 140 (14) (2014) 144107.
[107] K.T. Lundgaard, J. Wellendorff, J. Voss, K.W. Jacobsen, T. Bligaard, mBEEF-vdW: robust fitting of error estimation density functionals, Phys. Rev. B 93 (23) (2016) 235162.
[108] P. Pernot, The parameter uncertainty inflation fallacy, J. Chem. Phys. 147 (10) (2017) 104102.
[109] P. Pernot, B. Civalleri, D. Presti, A. Savin, Prediction uncertainty of density functional approximations for properties of crystals with cubic symmetry, J. Phys. Chem. 19 (2015) 5288−5304.
[110] S. De Waele, K. Lejaeghere, M. Sluydts, S. Cottenier, Error estimates for density-functional theory predictions of surface energy and work function, Phys. Rev. B 94 (23) (2016) 235418.
[111] J.D. McDonnell, N. Schunck, D. Higdon, J. Sarich, S.M. Wild, W. Nazarewicz, Uncertainty quantification for nuclear density functional theory and information content of new measurements, Phys. Rev. Lett. 114 (12) (2015) 122501.
[112] L. He, Y. Wang, An efficient saddle point search method using kriging metamodels, in: Proc. ASME 2015 International Design Engineering Technical Conferences and Computers and Information in Engineering Conference, August 2015 pp. V01AT02A008.
[113] G.N. Simm, M. Reiher, Error-controlled exploration of chemical reaction networks with Gaussian processes, J. Chem. Theory Comput. 14 (10) (2018) 5238−5248.

[114] X. Yang, H. Lei, P. Gao, D.G. Thomas, D.L. Mobley, N.A. Baker, Atomic radius and charge parameter uncertainty in biomolecular solvation energy calculations, J. Chem. Theory Comput. 14 (2) (2018) 759−767.
[115] F. Hanke, Sensitivity analysis and uncertainty calculation for dispersion corrected density functional theory, J. Comput. Chem. 32 (7) (2011) 1424−1430.
[116] J. Proppe, M. Reiher, Reliable estimation of prediction uncertainty for physicochemical property models, J. Chem. Theory Comput. 13 (7) (2017) 3297−3317.
[117] K.K. Irikura, R.D. Johnson, R.N. Kacker, Uncertainties in scaling factors for ab initio vibrational frequencies, J. Phys. Chem. A 109 (37) (2005) 8430−8437.
[118] K. Lejaeghere, V. Van Speybroeck, G. Van Oost, S. Cottenier, Error estimates for solid-state density-functional theory predictions: an overview by means of the ground-state elemental crystals, Crit. Rev. Solid State Mater. Sci. 39 (1) (2014) 1−24.
[119] K. Lejaeghere, G. Bihlmayer, T. Björkman, P. Blaha, S. Blügel, V. Blum, D. Caliste, I.E. Castelli, S.J. Clark, A. Dal Corso, S. De Gironcoli, etc, Reproducibility in density functional theory calculations of solids, Science 351 (6280) (2016) aad3000.
[120] F. Tran, J. Stelzl, P. Blaha, Rungs 1 to 4 of DFT Jacob's ladder: extensive test on the lattice constant, bulk modulus, and cohesive energy of solids, J. Chem. Phys. 144 (20) (2016) 204120.
[121] J.R. Rustad, D.A. Yuen, F.J. Spera, The sensitivity of physical and spectral properties of silica glass to variations of interatomic potentials under high pressure, Phys. Earth Planet. Inter. 65 (3) (1991) 210−230.
[122] M.I. Mendelev, S. Han, D.J. Srolovitz, G.J. Ackland, D.Y. Sun, M. Asta, Development of new interatomic potentials appropriate for crystalline and liquid iron, Philos. Mag. 83 (35) (2003) 3977−3994.
[123] S.B. Zhu, C.F. Wong, Sensitivity analysis of water thermodynamics, J. Chem. Phys. 98 (11) (1993) 8892−8899.
[124] T.D. Iordanov, G.K. Schenter, B.C. Garrett, Sensitivity analysis of thermodynamic properties of liquid water: a general approach to improve empirical potentials, J. Phys. Chem. 110 (2) (2006) 762−771.
[125] C.S. Becquart, C. Domain, A. Legris, J.C. Van Duysen, Influence of the interatomic potentials on molecular dynamics simulations of displacement cascades, J. Nucl. Mater. 280 (1) (2000) 73−85.
[126] S.L. Frederiksen, K.W. Jacobsen, K.S. Brown, J.P. Sethna, Bayesian ensemble approach to error estimation of interatomic potentials, Phys. Rev. Lett. 93 (16) (2004) 165501.
[127] F. Cailliez, P. Pernot, Statistical approaches to forcefield calibration and prediction uncertainty in molecular simulation, J. Chem. Phys. 134 (5) (2011) 054124.
[128] P. Angelikopoulos, C. Papadimitriou, P. Koumoutsakos, Bayesian uncertainty quantification and propagation in molecular dynamics simulations: a high performance computing framework, J. Chem. Phys. 137 (14) (2012) 144103.
[129] P. Angelikopoulos, C. Papadimitriou, P. Koumoutsakos, Data driven, predictive molecular dynamics for nanoscale flow simulations under uncertainty, J. Phys. Chem. B 117 (47) (2013) 14808−14816.
[130] F. Rizzi, H.N. Najm, B.J. Debusschere, K. Sargsyan, M. Salloum, H. Adalsteinsson, O.M. Knio, Uncertainty quantification in MD simulations. Part II: Bayesian inference of force-field parameters, Multiscale Model. Simul. 10 (4) (2012) 1460.
[131] R. Dutta, Z.F. Brotzakis, A. Mira, Bayesian calibration of force-fields from experimental data: TIP4P water, J. Chem. Phys. 149 (15) (2018) 154110.

[132] K. Farrell, J.T. Oden, D. Faghihi, A Bayesian framework for adaptive selection, calibration, and validation of coarse-grained models of atomistic systems, J. Comput. Phys. 295 (2015) 189−208.
[133] P.N. Patrone, T.W. Rosch, F.R. Phelan Jr., Bayesian calibration of coarse-grained forces: efficiently addressing transferability, J. Chem. Phys. 144 (15) (2016) 154101.
[134] L. Kulakova, P. Angelikopoulos, P.E. Hadjidoukas, C. Papadimitriou, P. Koumoutsakos, Approximate Bayesian computation for granular and molecular dynamics simulations, in: Proceedings of the ACM Platform for Advanced Scientific Computing Conference, 2016, p. 4.
[135] P.E. Hadjidoukas, P. Angelikopoulos, C. Papadimitriou, P. Koumoutsakos, Π4U: a high performance computing framework for Bayesian uncertainty quantification of complex models, J. Comput. Phys. 284 (2015) 1−21.
[136] F. Rizzi, H.N. Najm, B.J. Debusschere, K. Sargsyan, M. Salloum, H. Adalsteinsson, O.M. Knio, Uncertainty quantification in MD simulations. Part I: forward propagation, Multiscale Model. Simul. 10 (4) (2012) 1428.
[137] H. Lei, X. Yang, B. Zheng, G. Lin, N.A. Baker, Constructing surrogate models of complex systems with enhanced sparsity: quantifying the influence of conformational uncertainty in biomolecular solvation, Multiscale Model. Simul. 13 (4) (2015) 1327−1353.
[138] F. Cailliez, A. Bourasseau, P. Pernot, Calibration of forcefields for molecular simulation: sequential design of computer experiments for building cost-efficient kriging metamodels, J. Comput. Chem. 35 (2) (2014) 130−149.
[139] L.C. Jacobson, R.M. Kirby, V. Molinero, How short is too short for the interactions of a water potential? Exploring the parameter space of a coarse-grained water model using uncertainty quantification, J. Phys. Chem. 118 (28) (2014) 8190−8202.
[140] A.P. Moore, C. Deo, M.I. Baskes, M.A. Okuniewski, D.L. McDowell, Understanding the uncertainty of interatomic potentials' parameters and formalism, Comput. Mater. Sci. 126 (2017) 308−320.
[141] M.A. Tschopp, B.C. Rinderspacher, S. Nouranian, M.I. Baskes, S.R. Gwaltney, M.F. Horstemeyer, Quantifying parameter sensitivity and uncertainty for interatomic potential design: application to saturated hydrocarbons, ASCE-ASME J. Risk Uncertain. Eng. Syst. Part B Mech. Eng. 4 (1) (2018) 011004.
[142] R.A. Messerly, T.A. Knotts IV, W.V. Wilding, Uncertainty quantification and propagation of errors of the Lennard-Jones 12-6 parameters for n-alkanes, J. Chem. Phys. 146 (19) (2017) 194110.
[143] R.A. Messerly, S.M. Razavi, M.R. Shirts, Configuration-sampling-based surrogate models for rapid parameterization of non-bonded interactions, J. Chem. Theory Comput. 14 (6) (2018) 3144−3162.
[144] G. Dhaliwal, P.B. Nair, C.V. Singh, Uncertainty analysis and estimation of robust AIREBO parameters for graphene, Carbon 142 (2019) 300−310.
[145] A.V. Tran, Y. Wang, A molecular dynamics simulation mechanism with imprecise interatomic potentials, in: Proceedings of the 3rd World Congress on Integrated Computational Materials Engineering (ICME), John Wiley & Sons, 2015, p. 131.
[146] A.V. Tran, Y. Wang, Reliable Molecular Dynamics. Uncertainty quantification using interval analysis in molecular dynamics simulation, Comput. Mater. Sci. 127 (2017) 141−160.
[147] Reliable Molecular Dynamics. Available at: https://github.com/GeorgiaTechMSSE/.
[148] S. Plimpton, P. Crozier, A. Thompson, LAMMPS-large-scale Atomic/molecular Massively Parallel Simulator, Sandia National Laboratories, 2007.

[149] A. Tsourtis, Y. Pantazis, M.A. Katsoulakis, V. Harmandaris, Parametric sensitivity analysis for stochastic molecular systems using information theoretic metrics, J. Chem. Phys. 143 (1) (2014) 014116, 2015.
[150] S.T. Reeve, A. Strachan, Error correction in multi-fidelity molecular dynamics simulations using functional uncertainty quantification, J. Comput. Phys. 334 (2017) 207−220.
[151] P.N. Patrone, A. Dienstfrey, A.R. Browning, S. Tucker, S. Christensen, Uncertainty quantification in molecular dynamics studies of the glass transition temperature, Polymer 87 (2016) 246−259.
[152] K.S. Kim, M.H. Han, C. Kim, Z. Li, G.E. Karniadakis, E.K. Lee, Nature of intrinsic uncertainties in equilibrium molecular dynamics estimation of shear viscosity for simple and complex fluids, J. Chem. Phys. 149 (4) (2018) 044510.
[153] L. Alzate-Vargas, M.E. Fortunato, B. Haley, C. Li, C.M. Colina, A. Strachan, Uncertainties in the predictions of thermo-physical properties of thermoplastic polymers via molecular dynamics, Model. Simul. Mater. Sci. Eng. 26 (6) (2018) 065007.
[154] R.G. Ghanem, P.D. Spanos, Stochastic Finite Elements: A Spectral Approach, Courier Corporation, 1991.
[155] S. Sakamoto, R. Ghanem, Polynomial chaos decomposition for the simulation of non-Gaussian nonstationary stochastic processes, J. Eng. Mech. 128 (2) (2002) 190−201.
[156] C.C. Li, A. Der Kiureghian, Optimal discretization of random fields, J. Eng. Mech. 119 (6) (1993) 1136−1154.
[157] E. Vanmarcke, Random Fields, MIT Press, 1983.
[158] M. Grigoriu, Applied Non-gaussian Processes, Prentice Hall, 1995.
[159] M. Grigoriu, Random field models for two-phase microstructures, J. Appl. Phys. 94 (6) (2003) 3762−3770.
[160] L. Graham-Brady, X.F. Xu, Stochastic morphological modeling of random multiphase materials, J. Appl. Mech. 75 (6) (2008) 061001.
[161] J. Guilleminot, A. Noshadravan, C. Soize, R.G. Ghanem, A probabilistic model for bounded elasticity tensor random fields with application to polycrystalline microstructures, Comput. Methods Appl. Mech. Eng. 200 (17−20) (2011) 1637−1648.
[162] X. Yin, S. Lee, W. Chen, W.K. Liu, M.F. Horstemeyer, Efficient random field uncertainty propagation in design using multiscale analysis, J. Mech. Des. 131 (2) (2009) 021006.
[163] M. Shinozuka, G. Deodatis, Simulation of stochastic processes by spectral representation, Appl. Mech. Rev. 44 (4) (1991) 191−204.
[164] M.P. Mignolet, P.D. Spanos, Simulation of homogeneous two-dimensional random fields: Part I—AR and ARMA models, J. Appl. Mech. 59 (2S) (1992) S260−S269.
[165] B.A. Zeldin, P.D. Spanos, Random field representation and synthesis using wavelet bases, J. Appl. Mech. 63 (4) (1996) 946−952.
[166] W.K. Liu, T. Belytschko, A. Mani, Probabilistic finite elements for nonlinear structural dynamics, Comput. Methods Appl. Mech. Eng. 56 (1) (1986) 61−81.
[167] F. Yamazaki, M. Shinozuka, G. Dasgupta, Neumann expansion for stochastic finite element analysis, J. Eng. Mech. 114 (8) (1988) 1335−1354.
[168] I. Elishakoff, P. Elisseeff, S.A. Glegg, Nonprobabilistic, convex-theoretic modeling of scatter in material properties, AIAA J. 32 (4) (1994) 843−849.
[169] Y. Ben-Haim, I. Elishakoff, Convex Models of Uncertainty in Applied Mechanics, vol. 25, Elsevier, 2013.
[170] M.K. Deb, I.M. Babuška, J.T. Oden, Solution of stochastic partial differential equations using Galerkin finite element techniques, Comput. Methods Appl. Mech. Eng. 190 (48) (2001) 6359−6372.

[171] D. Xiu, J.S. Hesthaven, High-order collocation methods for differential equations with random inputs, SIAM J. Sci. Comput. 27 (3) (2005) 1118−1139.
[172] S. Huang, S. Mahadevan, R. Rebba, Collocation-based stochastic finite element analysis for random field problems, Probabilistic Eng. Mech. 22 (2) (2007) 194−205.
[173] B. Ganapathysubramanian, N. Zabaras, Modeling diffusion in random heterogeneous media: data-driven models, stochastic collocation and the variational multiscale method, J. Comput. Phys. 226 (1) (2007) 326−353.
[174] X. Ma, N. Zabaras, An adaptive hierarchical sparse grid collocation algorithm for the solution of stochastic differential equations, J. Comput. Phys. 228 (8) (2009) 3084−3113.
[175] H. Risken, The Fokker-Planck Equation: Methods of Solution and Applications, Springer, Berlin, 1996.
[176] S.A. Adelman, Fokker−Planck equations for simple non-Markovian systems, J. Chem. Phys. 64 (1) (1976) 124−130.
[177] V.S. Volkov, V.N. Pokrovsky, Generalized fokker−planck equation for non-markovian processes, J. Math. Phys. 24 (2) (1983) 267−270.
[178] M. Grigoriu, Non-Gaussian models for stochastic mechanics, Probabilistic Eng. Mech. 15 (1) (2000) 15−23.
[179] R.L. Bagley, P.J. Torvik, On the fractional calculus model of viscoelastic behavior, J. Rheol. 30 (1) (1986) 133−155.
[180] E. Lutz, Fractional Langevin equation, Phys. Rev. A 64 (5) (2001), 051106.
[181] S. Jespersen, R. Metzler, H.C. Fogedby, Lévy flights in external force fields: Langevin and fractional Fokker-Planck equations and their solutions, Phys. Rev. A 59 (3) (1999) 2736.
[182] M. Ostoja-Starzewski, J. Li, H. Joumaa, P.N. Demmie, From fractal media to continuum mechanics, ZAMM-J. Appl. Math. Mech. 94 (5) (2014) 373−401.
[183] T. Takaki, R. Rojas, S. Sakane, M. Ohno, Y. Shibuta, T. Shimokawabe, T. Aoki, Phase-field-lattice Boltzmann studies for dendritic growth with natural convection, J. Cryst. Growth 474 (2017) 146−153.
[184] X.B. Qi, Y. Chen, X.H. Kang, D.Z. Li, T.Z. Gong, Modeling of coupled motion and growth interaction of equiaxed dendritic crystals in a binary alloy during solidification, Sci. Rep. 7 (2017) 45770.
[185] H. Xing, X. Dong, J. Wang, K. Jin, Orientation dependence of columnar dendritic growth with sidebranching behaviors in directional solidification: insights from phase-field simulations, Metall. Mater. Trans. B 49 (4) (2018) 1547−1559.
[186] D. Liu, Y. Wang, Mesoscale multi-physics simulation of rapid solidification of Ti-6Al-4V alloy, Additive Manufacturing 25 (2019) 551−562.
[187] K. Fezi, M.J.M. Krane, Uncertainty quantification in modelling equiaxed alloy solidification, Int. J. Cast Metals Res. 30 (1) (2017) 34−49.
[188] A. Tran, D. Liu, H. Tran, Y. Wang, Quantifying uncertainty in the process-structure relationship for Al-Cu solidification, Model. Simul. Mater. Sci. Eng. 27 (2019) 064005.
[189] A. Karma, W.J. Rappel, Quantitative phase-field modeling of dendritic growth in two and three dimensions, Phys. Rev. A 57 (4) (1998) 4323.
[190] G. Da Prato, A. Debussche, Stochastic Cahn-Hilliard equation, Nonlinear Anal. Theory Methods Appl. 26 (2) (1996) 241−263.
[191] R.V. Kohn, F. Otto, M.G. Reznikoff, E. Vanden-Eijnden, Action minimization and sharp-interface limits for the stochastic Allen-Cahn equation, Commun. Pure Appl. Math. 60 (3) (2007) 393−438.
[192] G. Akagi, G. Schimperna, A. Segatti, Fractional Cahn−Hilliard, Allen−Cahn and porous medium equations, J. Differ. Equ. 261 (6) (2016) 2935−2985.

[193] Y. Wang, Multiscale uncertainty quantification based on a generalized hidden Markov model, J. Mech. Des. 133 (3) (2011) 031004.
[194] Y. Wang, D.L. McDowell, A.E. Tallman, Cross-scale, cross-domain model validation based on generalized hidden Markov model and generalized interval Bayes' rule, in: Proceedings of the 2nd World Congress on Integrated Computational Materials Engineering (ICME), Springer, 2013, pp. 149−154.
[195] A.E. Tallman, J.D. Blumer, Y. Wang, D.L. McDowell, Multiscale model validation based on generalized interval Bayes' rule and its application in molecular dynamics simulation, in: ASME 2014 International Design Engineering Technical Conferences and Computers and Information in Engineering Conference, 2014 pp. V01AT02A042.
[196] M. Schöberl, N. Zabaras, P.S. Koutsourelakis, Predictive coarse-graining, J. Comput. Phys. 333 (2017) 49−77.
[197] A.E. Tallman, L.P. Swiler, Y. Wang, D.L. McDowell, Reconciled top-down and bottom-up hierarchical multiscale calibration of bcc Fe crystal plasticity, Int. J. Multiscale Comput. Eng. 15 (6) (2017) 505−523.
[198] A.E. Tallman, L.P. Swiler, Y. Wang, D.L. McDowell, Hierarchical top-down bottom-up calibration with consideration for uncertainty and inter-scale discrepancy of Peierls stress of bcc Fe, Model. Simul. Mater. Sci. Eng. 27 (2019) 064004.
[199] L.J. Gosink, C.C. Overall, S.M. Reehl, P.D. Whitney, D.L. Mobley, N.A. Baker, Bayesian model averaging for ensemble-based estimates of solvation-free energies, J. Phys. Chem. B 121 (15) (2017) 3458−3472.
[200] R. Bostanabad, B. Liang, J. Gao, W.K. Liu, J. Cao, D. Zeng, X. Su, H. Xu, Y. Li, W. Chen, Uncertainty quantification in multiscale simulation of woven fiber composites, Comput. Methods Appl. Mech. Eng. 338 (2018) 506−532.
[201] M. Koslowski, A. Strachan, Uncertainty propagation in a multiscale model of nanocrystalline plasticity, Reliab. Eng. Syst. Saf. 96 (9) (2011) 1161−1170.
[202] H.J. Choi, R. Austin, J.K. Allen, D.L. McDowell, F. Mistree, D.J. Benson, An approach for robust design of reactive power metal mixtures based on non-deterministic micro-scale shock simulation, J. Comput. Aided Mater. Des. 12 (1) (2005) 57−85.
[203] A. Sinha, N. Bera, J.K. Allen, J.H. Panchal, F. Mistree, Uncertainty management in the design of multiscale systems, J. Mech. Des. 135 (1) (2013) 011008.
[204] T. Mukhopadhyay, A. Mahata, S. Dey, S. Adhikari, Probabilistic analysis and design of HCP nanowires: an efficient surrogate based molecular dynamics simulation approach, J. Mater. Sci. Technol. 32 (12) (2016) 1345−1351.
[205] P.C. Kern, M.W. Priddy, B.D. Ellis, D.L. McDowell, pyDEM: a generalized implementation of the inductive design exploration method, Mater. Des. 134 (2017) 293−300.
[206] D. Xue, P.V. Balachandran, J. Hogden, J. Theiler, D. Xue, T. Lookman, Accelerated search for materials with targeted properties by adaptive design, Nat. Commun. 7 (2016) 11241.
[207] T. Lookman, P.V. Balachandran, D. Xue, J. Hogden, J. Theiler, Statistical inference and adaptive design for materials discovery, Curr. Opin. Solid State Mater. Sci. 21 (3) (2017) 121−128.
[208] W. Chen, X. Yin, S. Lee, W.K. Liu, A multiscale design methodology for hierarchical systems with random field uncertainty, J. Mech. Des. 132 (4) (2010) 041006.
[209] S. Chen, W. Chen, S. Lee, Level set based robust shape and topology optimization under random field uncertainties, Struct. Multidiscip. Optim. 41 (4) (2010) 507−524.
[210] J. Zhao, C. Wang, Robust structural topology optimization under random field loading uncertainty, Struct. Multidiscip. Optim. 50 (3) (2014) 517−522.

[211] M. Tootkaboni, A. Asadpoure, J.K. Guest, Topology optimization of continuum structures under uncertainty−a polynomial chaos approach, Comput. Methods Appl. Mech. Eng. 201 (2012) 263−275.
[212] C.C. Seepersad, J.K. Allen, D.L. McDowell, F. Mistree, Robust design of cellular materials with topological and dimensional imperfections, J. Mech. Des. 128 (6) (2006) 1285−1297.
[213] J.K. Allen, C. Seepersad, H. Choi, F. Mistree, Robust design for multiscale and multidisciplinary applications, J. Mech. Des. 128 (4) (2006) 832−843.
[214] M. Schevenels, B.S. Lazarov, O. Sigmund, Robust topology optimization accounting for spatially varying manufacturing errors, Comput. Methods Appl. Mech. Eng. 200 (49−52) (2011) 3613−3627.
[215] P.D. Dunning, H.A. Kim, Robust topology optimization: minimization of expected and variance of compliance, AIAA Journal 51 (11) (2013) 2656−2664.
[216] N.P. Garcia-Lopez, M. Sanchez-Silva, A.L. Medaglia, A. Chateauneuf, An improved robust topology optimization approach using multiobjective evolutionary algorithms, Comput. Struct. 125 (2013) 1−10.
[217] J. Wu, Z. Luo, H. Li, N. Zhang, Level-set topology optimization for mechanical metamaterials under hybrid uncertainties, Comput. Methods Appl. Mech. Eng. 319 (2017) 414−441.

ELSEVIER SERIES IN **MECHANICS OF ADVANCED MATERIALS**

UNCERTAINTY QUANTIFICATION IN MULTISCALE MATERIALS MODELING

Edited by
YAN WANG AND DAVID L. MCDOWELL

Uncertainty Quantification in Multiscale Materials Modeling provides a complete overview of uncertainty quantification (UQ) in computational materials science. It provides practical tools and methods along with examples of their application to problems in materials modeling. UQ methods are applied to various multiscale models ranging from the nanoscale to macroscale. This book presents a thorough synthesis of the state-of-the-art in UQ methods for materials modeling, including Bayesian inference, surrogate modeling, random fields, interval analysis, and sensitivity analysis, providing insight into the unique characteristics of models framed at each scale, as well as common issues in modeling across scales.

Key features

- Synthesizes available UQ methods for materials modeling
- Provides practical tools and examples for problem solving in modeling material behavior across various length scales
- Demonstrates UQ in density functional theory, molecular dynamics, kinetic Monte Carlo, phase field, finite element method, multiscale modeling, and to support decision making in materials design
- Covers quantum, atomistic, mesoscale, and engineering structure-level modeling and simulation

ISBN 978-0-08-102941-1
9 780081 029411

ELSEVIER elsevier.com/books-and-journals