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Preface for Focus Issue on Uncertainty Quantification in Materials Modeling

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This focus issue is motivated by the growing demand for rigorous uncertainty quantification (UQ) in materials modeling, which is driven by the need to use these tools, in conjunction with experiments, to support decision making in materials design, development, and deployment. Traditionally, predictive materials modeling has focused on gaining qualitative insight into the range of mechanisms that control material behavior and how those mechanisms interact to govern material properties and processes. In that context, quantitative evaluation of modeling uncertainty was not a priority. As materials modeling advances, there is increased impetus to employ it in the context of materials design and qualification. This trend is manifested in the establishment of Integrated Computational Materials Engineering (ICME) as a growing sub-discipline, as well as by initiatives such as the Materials Genome (MGI) in the USA and similar efforts around the globe. Current practice and future needs are described in several recent reports including NASA's *Vision 2040: A Roadmap for Integrated, Multiscale Modeling and Simulation of Materials and Systems*. Invariably, these studies point out the need for the field to embrace the challenge of UQ.

The selected articles for this MSMSE Focus Issue summarize the current state of this field and identify important opportunities and needs. They also highlight unique challenges facing the materials community with respect to UQ, including the use of approximate physics, model form uncertainty, and uncertainty across scales. The goal of this collection of articles is to stimulate research in this area, serve as useful reference to the community, and to promote a cultural change so that treatment of uncertainty becomes a routine aspect of materials modeling. We next summarize these articles by logical groupings.

Digital datasets for materials are becoming increasingly available to the materials community and present unique challenges. ***Jha et al.*** address the important challenge of dealing with uncertainties in large materials datasets and specifically managing them when developing surrogate models using machine learning techniques.

Two contributions focus on UQ in the context of additive manufacturing driven by the need of quality control. ***Nath et al.*** discuss uncertainties in grain morphology in laser direct metal deposition, a description that requires a multiscale approach. The authors use a combination of finite element modeling to describe the melt pool and cellular autonoma techniques for crystallization; they introduce surrogate models to replace computationally intensive simulations, thereby adding complexity to the UQ analysis. ***Gosh et al.*** focus on microsegregation

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and also using a multiscale approach quantify the role of several variables on their quantities of interest. This information can be used to refine processes and in materials selection. In a related contribution, ***Tran et al.*** address solidification in Al-Cu alloys. Using a surrogate model based on phase field simulations to quantify how processing and thermodynamic parameters affect several quantities of interest, including dendrite geometry.

Two contributions address challenges in atomistic simulations that originate from the selection of interatomic potentials. ***Ragasa et al.*** describe an approach to deal with the challenge of multi-objective optimization in the development of interatomic potentials. They use machine learning techniques to identify an ensemble of interatomic potentials that lie of the Pareto front of error space. Each member of the ensemble is optimal in that the error in any of the training properties cannot be improved without increasing the error on a different target. ***Reeve et al.*** focus on the related problem of quantifying uncertainties in atomistic simulations originating from the interatomic potential used, importantly addressing the effect of the actual function as opposed to model parameters. This contribution extends functional uncertainty quantification (FunUQ) to new quantities of interest and simulation conditions, demonstrating that predictions for a new interatomic potential can be made without re-running the simulations under certain conditions.

Calibration of model parameters for models addressing a given length scale of interest is complicated when some information is obtained by lower scale simulations (e.g., atomistic modeling) and higher scale experiments, both routes having errors and associated uncertainty. ***Tallman et al.*** address a novel combined top-down and bottom-up strategy to consider a constrained maximum likelihood scheme to estimate model parameters for crystal plasticity of bcc Fe that reconcile both pathways. This is accomplished by adding a model discrepancy layer that involves activation of Frank-Read dislocation sources at the mesoscale. Another paper by ***Honarmandi et al.*** considers UQ in calibrating parameters of models for the behavior of shape memory alloys that undergo thermally induced phase transformation. They carry out Bayesian Markov Chain Monte Carlo analyses and propagate uncertainties in the calibrated model parameters using a relevant sampling technique to predict confidence intervals for predicted responses.

To address uncertainty in alloy design owing to variation of composition, ***Müller et al.*** discuss a fast model that mitigates variability of composition by seeking compositions that are robust against such variation. This is accomplished by employing a regression-based model for calculating the sensitivity that only requires one-time calculation of the regression coefficients. The model is then successfully applied to the computational alloys-by-design workflow to facilitate alloy selection using the sensitivity of a composition owing to the inaccuracies in the manufacturing process as an additional minimization goal.

We trust that the readers of this Focus Issue on Uncertainty Quantification in Materials Modeling will benefit from the range of UQ techniques and applications presented, and will gain new appreciation of the both the challenges and opportunities facing this important emerging field.

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