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Furnas 206**

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Data-enabled Predictive Modeling of Advanced Manufacturing of Materials

ABSTRACT

The dramatic advances in computational and computer science over the last two decades have enabled the scientific community to push the prediction capabilities of computational models. Consequently, the development of computational models of complex materials systems, to new heights complimented by experimental data, can positively impact quantitative outcomes of advanced manufacturing of novel materials and potentially speed up the transition from the research laboratory to the commercial manufacturing process. Implicit in predictive modeling of materials systems is the employment of supervised learning algorithms to train the computational models (calibration) and challenge their predictable capabilities (validation) against sets of training and test data, while coping with inevitable uncertainties in the model parameters and noisy and incompleteness of experimental measurements. The problem of overriding importance is to characterize all of these uncertainties, assessing the reliability of computational prediction, and to ultimately conduct meaningful decision under uncertainty.

This talk is centered on developing and implementing theories, data-driven methods, and computational tools to address important challenges in computational materials engineering and their applications to predictive modeling of advanced manufacturing of materials. This involves development of physics-based models of metallic microsystems, in the context of the enhanced (nonlocal) continuum mechanics, that extend the time and length scales of classical theories. Then, a general data-driven framework, based on the Occam Plausibility Algorithm (OPAL) concept, is discussed that allows integration of observational data and computational models while addressing uncertainties in parameters, data, and model selection. Using Bayesian machine learning and information theoretics, OPAL systematically assesses and propagates uncertainties through models at multiple scales, while accounting for the trade-off between validity and complexity of models. The implementation of this framework, for coarse-grained models and atomistic systems is presented. Future research directions, including material design under uncertainty are also discussed.

BIO SKETCH

Danial Faghihi is a Research Associate at the Institute for Computational Engineering and Science (ICES) in the University of Texas at Austin. He graduated with a PhD degree in civil engineering from Louisiana State University in December 2012 and worked under the supervision of Boyd Professor George Z. Voyiadjis on theoretical and computational nonlinear and nonlocal continuum solid mechanics and finite elements methods. In January of 2013, Dr. Faghihi joined University of Texas at Austin as a post-doctoral fellow at ICES working with Professor J. Tinsley Oden on statistical and computational methods for predictive modeling of complex physical system with quantified uncertainties. His research interests include multiscale material modeling, Bayesian machine learning, and data-enabled predictive science with applications to advanced manufacturing of materials and other complex physical systems.



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