

DEPARTMENT OF MECHANICAL ENGINEERING

WILLIAM MAXWELL REED SEMINAR SERIES

“Multiscale Modeling of Materials: Uncertainty Quantification and Goal-Oriented Optimization”

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Abstract: The macroscopic properties of materials and structures that we observe and exploit in engineering applications result from complex interactions between physics at multiple length and time scales: electronic, atomistic, defects, domains, etc. Multiscale modeling seeks to understand the interactions between these physics across scales. However, assessing such interactions can be challenging due to the complex nature of material properties and the prohibitive computational cost of integral calculations. This talk focuses on the essential problems of interactions along two scaling directions in the multiscale modeling: uncertainty quantification (upscaling) and goal-oriented optimization (downscaling). First, we exploit the multiscale and hierarchical nature of material response and develop a framework to quantify the overall uncertainty of material response induced by the uncertainties at finer scales without the need for integral calculations. Specifically, we bound the uncertainty at each scale and then combine the partial uncertainties in a way that provides a bound on the overall or integral uncertainty. The bound provides a conservative estimate on the uncertainty. Importantly, this approach does not require integral calculations that are prohibitively expensive. The second part of the talk will focus on the optimization of material performance over multiple properties across scales. We develop a joint co-optimization framework, in which the material is regarded as a whole system and the design of material is formulated as a constrained optimization problem that is solved over all the design parameters simultaneously, including both mechanical and structural properties. The design objective is to maximize a crucial metric that characterizes the targeted performance of the material in the application. This approach takes into account not only the connection between components, but also the connection between the entire material and its application environments. This talk will also show the demonstration of the two frameworks in the applications of high-speed impact of AZ31B magnesium alloy and polyurea plates.

Bio: Dr. Xingsheng Sun is a Postdoctoral Scholar in Aerospace at California Institute of Technology, working with Prof. Michael Ortiz and Prof. Kaushik Bhattacharya. His research background includes computational solid mechanics, uncertainty quantification, inverse problems, and high-performance computing. His main research interest lies in multiscale quantification of material uncertainties, application-driven materials by design, mechanics of materials in extreme conditions, and long-term atomistic modeling and simulations. Dr. Sun holds a Ph.D. degree in Aerospace Engineering from Virginia Tech, and his thesis advisor is Prof. Kevin Wang. He received his B.S. degree from Dalian University of Technology (China) and his M.S. degree from Hunan University (China), both in Mechanical Engineering.

Date: Friday, Apr. 16th

Place: <https://uky.zoom.us/j/92940732923>

Time: 1:00PM EST

Contact: Dr. Alexandre Martin 257-4462

Attendance open to all interested persons