Symposium | A. Advances in Materials Theory for Multiscale Modeling

[SY-A4]Symposium A-4

Chair: David L McDowell(Woodruff School of Mechanical Engineering, Georgia Institute of Technology, United States of America)

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[SY-A4]Modeling microstructural material variability with uncertainty quantification and machine learning techniques

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Material variability from heterogeneous microstructure, such as grain and pore morphologies, can have significant effects on component behavior and creates uncertainty around performance. Current engineering material models typically do not incorporate microstructural variability explicitly, rather functional forms are chosen based on intuition and parameters are selected to reflect mean behavior. Conversely, mesoscale models that capture the microstructural physics, and inherent variability, are impractical to utilize at the engineering scale. An enhanced design methodology must be developed for materials with significant variability, such as current additively manufactured (AM) metals, to predict the ensemble response.

To address these challenges we have developed a method based on the Embedded Uncertainty formulation, Sargsyan, Najm, Ghanem (2015) to calibrate distributions of material parameters from high-throughput experimental data. With this method, material variability is directly associated with commonly-used material parameters using a chosen nominal model. One of the benefits of this approach is that expert knowledge can be extended to interpret the effect of (hidden) microstructure on variable mechanical response. In a complementary effort, we are developing machine learning techniques to handle the large volume of data from high-throughput methods. The focus of this aspect is on adapting common machine learning models, such as neural networks, to obey the same exact properties and symmetries as traditional constitutive models while representing features in the data in a flexible, bias-less manner, Tensor Basis Neural Network in Ling, Jones, Templeton (2016). Classical constitutive modeling provides guidance in selecting appropriate microstructural descriptors as inputs and functional frameworks for outputs. Examples of application of these techniques to polycrystalline, porous metals, motivated by current AM materials, will be given.