Mechanistic data-driven design of complex multiscale material systems

Wing Kam Liu

PhD, PE, Walter P. Murphy Professor, Northwestern University
President of the International Association for Computational Mechanics
Chair, US National Committee on Theoretical & Applied Mechanics within the US National Academies
Member of the US Board of International Scientific Organizations within the US National Academies
http://www.tam.northwestern.edu/wkl/liu.html, w-liu@northwestern.edu

The advent of advanced processing and manufacturing techniques provides unparalleled freedom to design new material classes with complex microstructures across scales from nanometers to meters. In this lecture a new data-driven computational framework for the design of these complex material systems will be presented. A mechanistic multiscale method called self-consistent clustering analysis (SCA) is developed for general inelastic heterogeneous material systems. The efficiency of SCA is achieved via using data compression algorithms to group local microstructures into clusters during the off-line training stage, and its accuracy is guaranteed by introducing a self-consistent method for solving the Lippmann-Schwinger integral equation in the on-line predicting stage. Then the integration of microstructure reconstruction and subsequent high-fidelity multiscale predictions of the materials behavior leads to the generation of vast amounts of reliable data. Based on the computational design of experiments, data mining techniques offer the ability to discover the influence of the microstructure on the macroscopic materials behavior. This process-property-structure-performance feedback loop enables the design of new material systems with new capabilities. The proposed framework is illustrated for advanced composites and the integrated design of various advanced material systems, from additive manufactured material systems to soft matters and energy harvesting metamaterials.