

Self Consistent Clustering Theory for Failure Prediction of multiscale materials

A predictive computational theory is shown for modeling complex, hierarchical materials ranging from metal alloys to polymer nanocomposites. The theory can capture complex mechanisms such as plasticity and failure that span across multiple length scales. This general multiscale material modeling theory relies on sound principles of mathematics and mechanics, and a cutting-edge reduced order modeling method named self-consistent clustering analysis (SCA) [Zeliang Liu, M.A. Bessa, Wing Kam Liu, "Self-consistent clustering analysis: An efficient multi-scale scheme for inelastic heterogeneous materials," *Comput. Methods Appl. Mech. Engrg.* 306 (2016) 319–341]. SCA reduces by several orders of magnitude the computational cost of micromechanical and concurrent multiscale simulations, while retaining the microstructure information. This remarkable increase in efficiency is achieved with a data-driven clustering method. Computationally expensive operations are performed in the so-called offline stage, where degrees of freedom (DOFs) are agglomerated into clusters. The interaction tensor of these clusters is computed. In the online or predictive stage, the Lippmann-Schwinger integral equation is solved cluster-wise using a self-consistent scheme to ensure solution accuracy and avoid path dependence. To construct a concurrent multiscale model, this scheme is applied at each material point in a macroscale structure, replacing a conventional constitutive model with the average response computed from the microscale model using just the SCA online stage. A regularized damage theory is incorporated in the microscale that avoids the mesh and RVE size dependence that commonly plagues microscale damage calculations. The SCA method is illustrated with two cases: a carbon fiber reinforced polymer (CFRP) structure with the concurrent multiscale model and an application to fatigue prediction for additively manufactured metals. For the CFRP problem, a speed up estimated to be about 43,000 is achieved by using the SCA method, as opposed to FE^2 , enabling the solution of an otherwise computationally intractable problem. The second example uses a crystal plasticity constitutive law and computes the fatigue potency of extrinsic microscale features such as voids. This shows that local stress and strain are captured sufficiently well by SCA. This model has been incorporated in a process-structure-properties prediction framework for process design in additive manufacturing.