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Fully coupled multiscale modeling of cohesive failure in heterogeneous interfaces using high performance computing

Mosby, Matthew, mmosby1@nd.edu; Matous, Karel, University of Notre Dame, United States

ABSTRACT

Multiscale interfaces are prevalent throughout engineering design and application, often in the form of layered composites and adhesive joints. Most modern adhesives are highly heterogeneous, containing a wide range of sizes, shapes, and material properties of reinforcing constituents. Predicting how the size, shape, orientation, and distribution of the reinforcing particles change the failure response of the bonded structure is important for design and safety assessment. Using Direct Numerical Modeling to predict the failure of engineering-scale bonded structures is often too computationally expensive, even for today's supercomputers. Therefore, we have developed a hierarchically parallel numerical framework using Computational Homogenization (CH) to compute the multiscale failure response of heterogeneous interfaces in the 3D finite strain setting. The CH framework assumes a separation scales, and locally attaches a Representative Unit Cell (RUC) of the microstructure to each macroscopic point on the interface. The response of the different scales is linked through the variational energy equivalence (Hill's Lemma) for interfaces. The macroscopic cohesive law is thereby computationally derived with no assumption of its functional form. We present three-dimensional microscale simulations that resolve the large range of spatial scales, from the failure-zone thickness up to the size of the RUC, in damage mechanics problems of particle reinforced adhesives. We show that resolving this wide range of scales in complex three-dimensional heterogeneous morphologies is essential to apprehend fracture characteristics. Moreover, we show that computations that resolve the essential physical length-scales of the problem capture the particle size-effect in fracture toughness, for example. These simulations are computationally expensive and highlight the need for high-performance computing. To overcome the large computational burden of modeling the failure of bonded systems, we have developed a verified, highly scalable, hierarchically parallel client-server CH framework that uses our high-performance finite element solver to simultaneously compute both the macro- and microscales. We present fully coupled multiscale simulations resolving from O(10) nm to O(10) mm (O(106) length scales) requiring over 1 billion elements computed using fewer than 2000 processing cores. Fully coupled multiscale simulations of interfacial failure including matrix tearing and particle-matrix debonding are also presented.