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Predictive Modelling of Materials Failure Processes

Abstract

Fracture is the dominant failure process underlying many materials reliability issues. At the same time, it remains one of the most challenging 'multi-scale' modelling problems, requiring both an accurate description of the chemical processes occurring in the near tip region and the inclusion of a much larger region in the model systems. These requirements can be met simultaneously by combining a quantum mechanical description of the crack tip with a classical atomistic model that captures the long-range elastic behaviour of the surrounding crystal matrix in the "Learn on the Fly" (LOTF) approach. The approach has been successfully applied to simulation fracture behaviours in a number of systems, yielding predictions in excellent agreement with experiment. A recent Machine Learning reformulation of LOTF stores all QM calculations in a database which can then be used to predict forces on new configurations, reducing the need for expensive calculations. Planned future work involves consideration of how information obtained from predictive QM simulations can be efficiently coarse grained to provide input into continuum models including explicit uncertainty quantification, and how on-the-fly machine learning could be applied to improve the computational efficiency of other multiscale materials simulation methods.