Coupled Atomistics and Discrete Dislocations in 3d (CADD-3d)

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Capturing plasticity at realistic dislocation densities with high configurational complexity requires a continuum-level discrete dislocation dynamics (DDD) description. However, many features controlling dislocation motion are inherently atomistic, such as the interaction of dislocations with solutes, precipitates, cracks, and interfaces. Here, we present an approach to achieving a multiscale concurrent coupled atomistics/discrete-dislocation model in 3d (CADD3d), using the DDD code Paradis and the MD code LAMMPS. In CADD3d, dislocations can be described with atomistic resolution in one spatial domain that is fully and intimately coupled to a surrounding continuum domain in full 3d, with individual dislocation lines spanning *both* domains simultaneously. The need for precise matching of continuum dislocation properties to atomistic dislocation properties is demonstrated, and issues in making this connection are also discussed. Implementation of the model is presented, and several validation problems are present to demonstrate the robustness of the model for near-seamless motion of dislocations into, across, and out of the atomistic domain.

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