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A Novel Atomistic-Continuum Coupling Method for Amorphous Polymers at Finite Temperature

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In this work, a new simulation technique is presented for the concurrent mechanical coupling of particle and continuum domains at finite temperatures with potential application to fracture simulation in polymer nanocomposite materials. The coupling methodology is based on the Arlequin framework as proposed by Ben Dhia et al. for particle-continuum coupling in [1] and utilizes the concept of so-called anchor points for transmitting information between the two domains as developed in [2]. A bridging domain is defined wherein the particle and continuum domains overlap and forces and displacements may be transmitted. The present work draws upon the idea of grouping particles in the bridging domain to form Interface Volume Cells (IVC) as presented in [3]. These groups of atoms are then, in a spatially and temporarily averaged sense, connected by springs to respective anchor points in the continuum domain. This combination of techniques results in a new formulation that circumvents the need to connect continuum anchor points to individual particles, while benefitting from the inherent stability of a tunable spring-based load transfer mechanism.

In the present work, the particle domain is modelled using Molecular Dynamics (MD) in an all-atom representation at a temperature of 300 K and the continuum domain is modelled using the Finite Element Method (FEM). The two domains are solved iteratively until convergence is achieved for a given load state. Due to the continuum and particle domain time scales being vastly different, the FEM domain is solved statically, while the MD domain is run dynamically. A static uniaxial tension test is simulated using a three-dimensional block of EPON-862 resin, that is 85% crosslinked with curing agent DETDA. The applied loading is initially maintained within the linear elastic regime for model verification. Quantities such as stresses, Young's modulus, Poisson's ratio, and reaction forces are analyzed for convergence in the bridging domain and verified against a similar specimen modelled fully with FEM using experimental data available for EPON-862. After model verification in the linear elastic range, the loading is increased to simulate damage evolution and failure localization in the MD domain, in order to verify the post-yield behavior of the coupled model.

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