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From Nano to Micro by Computational Homogenization: A Static--Implicit Finite Element Coupling to Molecular Statics

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Abstract

We formulate a two-scale, nano-to-micro computational homogenization method that lifts atomistic accuracy to micro-meter structures. In contrast to micro--macro couplings, the upper scale here is the microscale (structures of order micro-m), while the lower scale is a nanoscale representative volume element (RVE) solved by molecular statics. The scale transition is carried out following Hill's macrohomogeneity principle based on power-conjugate pairsl The micro problem (finite elements) is posed in the work-conjugate pair of the 2nd Piola-Kirchhoff stress tensor and the Green-Lagrange strain tensor for finite strains. Nanoscale stresses are obtained from LAMMPS as volume-averaged Cauchy stresses and are consistently rotated and pulled back to the 2nd P.K. The required micro-scale tangent is built by forward differences of symmetric perturbations of the right stretch tensor from the polar decomposition. Because the micro finite element formulation employs a geometrically nonlinear total-Lagrangian setting, the consistent tangent comprises a material part and an initial-stress (geometric) part. The approach is material-agnostic at the nano scale; we showcase embedded-atom method (EAM) potentials for fcc metals in descriptive examples

Keywords:

multiscales homogenization atomic-to-continuum