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On The Nonlinear Mechanics of Carbon Nanocones Using The Consistent Atomic-scale Finite Element Method ARASH MAHDAVI, Penn State, Department of Mechanical and Nuclear Engineering, ERIC MOCKENSTURM, Penn Sate, Department of Mechanical and Nuclear Engineering — In the present work, a new multiscale modeling technique called the Consistent Atomic-scale Finite Element (CAFÉ) method is introduced. Unlike traditional approaches for linking the atomic structure to its equivalent continuum, this method directly connects the atomic degrees of freedom to a reduced set of finite element degrees of freedom without passing through an intermediate homogenized continuum. As a result, there is no need to introduce stress and strain measures at the atomic level. The Tersoff-Brenner interatomic potential is used to calculate the consistent tangent stiffness matrix of the structure. In this finite element formulation, all local and non-local interactions between carbon atoms are taken into account using overlapping finite elements. In addition, a consistent hierarchical finite element modeling technique is developed for adaptively coarsening and refining the mesh over different parts of the model. This process is consistent with the underlying atomic structure and, by refining the mesh, molecular dynamic results will be recovered. In contrast with most other multiscale methods, there is no need to introduce artificial boundaries for coupling atomistic and continuum regions. The applicability of the method is shown with several examples of deformation of carbon nanocones subjected to different loads and boundary conditions.

Arash Mahdavi
Penn State

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