A Dynamic Model Reduction Technique for the Multi-scale Modeling of Carbon Nanostructures

A new multi-scale 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 to the scale of atomic spacing, molecular dynamic results will be recovered. This method is valid across the scales and can be used to concurrently model atomistic and continuum phenomena so, in contrast with most other multi-scale methods, there is no need to introduce artificial boundaries for coupling atomistic and continuum regions. Effect of the length scale of the nanostructure is also included in the model by building the hierarchy of elements from bottom up using a finite-size atom cluster as the building block. To be consistent with the Bravais multi-lattice structure of sp^2-bonded carbon, two independent displacement fields are used for reducing the order of the model. Applicability of the method is shown with several examples of the nonlinear mechanics of graphene sheets, carbon nanotubes, and carbon nanocones subject to different loadings and boundary conditions.