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Atomistic-to-continuum coupling based on goal-oriented adaptivity and quasi-continuum approximation

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ABSTRACT

It has long been understood that some of the key characteristics of materials, like grain boundaries, dislocation cores, and crack tips cannot be modeled realistically within the framework of continuum mechanics. It is believed that defects and surface effects play important roles at small scales, where the continuum assumptions are violated. Therefore, further information on a material at its atomic scale is required to give a more physically based description of the phenomena governing the macroscopic behavior. A well-established method for concurrent coupling between atomistic and continuum regions is the quasi-continuum (QC) method. Basically, it relies on the fact that in many practical cases, only a small region in the material needs to be modeled atomistically. As a result, the assumptions of continuum mechanics can still be adopted for modeling the remaining regions without loss of the accuracy. This strategy provides a significant gain in computational cost, whereas the interesting phenomena pertaining to the atomistic area are also preserved. In this study, atomistic-to-continuum homogenization of molecular statics problem has been advanced with particular focus on the effect of lattice defects. A representative unit lattice (RUL) with Cauchy–Born boundaries is considered for obtaining homogenized response of the graphene lattice in terms of membrane forces (macroscale stress). In order to facilitate such an analysis, an adaptive strategy based on goal-oriented error estimation is developed for retaining the accuracy in the “goal-quantity” or “quantity of interest”, chosen to be the macroscale (continuum) stress. The QC method is introduced in two steps. First, we consider the restriction of atom displacement in terms of the representative atoms as a model reduction. The second step in the QC method is that of quadrature. For large QC elements, i.e., for a large amount of atoms whose placements are governed by the same representative atoms, the bond energy and its derivatives are typically computed using an appropriate discrete quadrature. We show how cluster approximation generates a quadrature error (in addition to the discretization error). Error because of different sources, namely: interpolation and quadrature parts of the QC method is approximated by solving the pertinent dual (adjoint) problem relevant to the output of interest. A hierarchical strategy is proposed for approximating the residual on an intermediate mesh, thus avoiding high computational cost that pertains to solving the full system. Homogenization of the macroscale membrane forces, including initial relaxation, is considered for the graphene in presence of divacancy defect. The Carbon–Carbon interactions are modeled via the Tersoff–Brenner potential enabling computation of bond energies up to the next nearest neighbor. The reliability of the adaptive algorithm is demonstrated through the numerical simulations on the respective RUL under macroscopic deformation.Further, we present an extension of the coupling methodology by developing strategies to obtain a macroscopically relaxed RUL. The RUL with Cauchy–Born boundaries is relaxed in a (nested) iterative procedure so that the macroscopic stress becomes zero for a certain equilibrium configuration. A stress–strain (i.e., membrane forces) response originating from macroscopically relaxed configuration is derived in two steps. The first step results in a stress-free configuration by finding a deformation map that corresponds to zero effective stress response. The subsequent step involves a multiplicative decomposition of the deformation and the pertinent push-forward of the effective stress.