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GOAL-ORIENTED ERROR CONTROL FOR THE QUASI CONTINUUM METHOD

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Abstract. In order to consider virtual materials (not physically manufactured) or in order to predict complex behavior on one length scale where the physics is better understood on a lower scale, homogenization (or coarse-graining) can be a useful tool. Considering atomistic systems, homogenization can be used to derive continuum properties whereby the need for empirical continuum models i avoided. When there is a large separation of scales, i.e. when the length scales of the sought continuum solution by far exceeds the atomistic length scale, computational homogenization can be adopted, see e.g. [1]. Using this approach, the continuum stress-strain response can be obtained implicitly by considering a representative volume element (RVE), also called representative lattice unit in the case of a homogenization of a discrete lattice. However, when considering atomistic systems, it is well known that defects play an important role. When investigating the influence from single (or a few) defects, very large RVE's need be considered.

In the case of scale-mixing, i.e. when the continuum scale and the atomistic scale needs be resolved concurrently in the spatial domain, one popular method is the Quasi-Continuum (QC) method, cf. [2, 3]. It allows for coarse graining of atomistic response in terms of interpolation on a "finite-element-type" mesh. The QC method is an approximation of the atomistic problem, rather than a homogenization technique.

In this contribution we establish the RVE for carrying out atomistic-to-continuum homogenization of a molecular statics problem. In particular, we are interested in computing the representative response for different imperfections in a lattice. To this end, we wish to consider relatively large lattices on the atomistic scale. In order to facilitate such an analysis, we proceed along the lines of, e.g., [4] and device a goal-oriented adaptive QC procedure for solving the atomistic problem on the RVE. Within the goal-oriented framework it becomes natural to consider the macro scale (continuum) stress as the goal-quantity that is solved for.

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, i.e., we describe the positions of all atoms in terms of discrete weights and the placements of certain so-called representative atoms. Based on this approximation, while accounting for the exact summation of all the bond-energies, we are able to compute goal-oriented error estimators in a straight-forward fashion based on an adjoint (dual) problem pertaining to the chosen output of interest. This computable error estimator pertains to a discretization error in the finite element method. 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 this approximation generates a quadrature error (in addition to the discretization error) in the framework for error estimation presented above. The combined error is estimated approximately based on the same dual problem in conjunction with a hierarchical strategy for approximating the residual.

As a model problem, we consider a mono-layer of graphene. The homogenization of the macro-scale membrane forces, including initial relaxation, is considered for defective graphene lattices. The 0 Kelvin condition is considered by omitting lattice vibration and the Carbon-Carbon energy bonds are modeled via the Tersoff-Brenner potential, cf. [5], which involves next-nearest neighbor couplings. In particular, we study the accuracy and robustness of the proposed error estimator and the pertinent adaptive algorithm.

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