Coarse-Grained Atomistics Via Meshless and Mesh-Based Quasicontinuum Techniques

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ABSTRACT

Spatial coarse-graining techniques are powerful methods to overcome the computational limits of molecular dynamics. In order to extend atomistic simulations of crystalline materials to the micron-scale and beyond, the quasicontinuum (QC) approximation [1-3] reduces large crystalline atomistic ensembles to a significantly smaller number of representative atoms with suitable interpolation schemes to infer the motion of all particles. In contrast to most other concurrent multiscale techniques, this allows for the simulation of large systems solely based on interatomic potentials and thus without the need for (oftentimes phenomenological) continuum constitutive models. This promises superior accuracy for predictive simulations at the meso- and macroscales.

Here, we will discuss one such coarse-graining scheme, viz. a fully-nonlocal energy-based QC technique [4,5] which excels by minimal approximation errors and vanishing force artefacts (a common problem in concurrent scale-coupling methods) [6]. Our model is equipped with automatic adaptation techniques to effectively tie atomistic resolution to regions of interest while efficiently coarse-graining the remaining solid. We review both mesh-based [6] and meshless formulations [4]. The former adopts methods from finite elements (using an affine interpolation on a Delaunay triangulation), whereas the latter is based on local maximum-entropy interpolation schemes. In both cases, the result is a computational toolbox for coarse-grained atomistic simulations, whose computational challenges are quite similar to those of molecular dynamics. Finite temperature extensions as well as coarse-graining in time can be incorporated in the presented framework [7].

We will review the underlying theory and give an overview of the state of the art, followed by a suite of numerical examples demonstrating the benefits and limitations of the nonlocal energy-based QC method. Examples range from nanoindentation and material failure to defect interactions and nanoscale mechanical size effects.

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