Multiscale Design of Advanced Materials by the Quasicontinuum Method: Mathematical Validation, Algorithms, and Applications

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Summary

The atomistic structure of crystalline materials is nearly periodic in space except for small regions around defects. The quasicontinuum (QC) approximation can significantly reduce the number of computational degrees of freedom by using atomistic models only in the regions around defects and continuum models elsewhere. We have developed a computable estimate for the modeling error and a corresponding adaptive algorithm to reliably select which regions need the accuracy of atomistic modeling to achieve a required error tolerance. We are also extending QC from crystals with a simple lattice structure to more complex materials including silicon, ferroelectrics, shape memory alloys, materials with chemistry, and objective structures such as carbon nanotubes, viral capsids and many viral parts (necks, tails, baseplates), and many of the common proteins (actin, collagen GroEL, hemoglobin).

The quasicontinuum (QC) method uses finite element interpolation and the locality assumption of continuum mechanics to efficiently approximate large parts of a material surrounding an atomistic region of interest (see Fig 1). The atoms underlying the continuum region are assumed to move according to the continuum field, an approximation referred to as *Cauchy-Born* kinematics. Our research focuses on establishing a rigorous mathematical foundation for QC, while continuing to extend the capabilities of this approach.

We have developed and analyzed a goal-oriented a posteriori error estimator for the atomistic-continuum modeling error in the QC method. Based on this error estimator, we have developed an algorithm which adaptively determines which regions need to be modeled atomistically to be able to compute a quantity of interest to within a given tolerance. We have applied the algorithm to the computation of the structure of a crystallographic defect described by a Frenkel-Kontorova model and obtained numerical results that show that our method gives an effective estimate of the error and a nearly optimal atomistic-continuum modeling strategy.

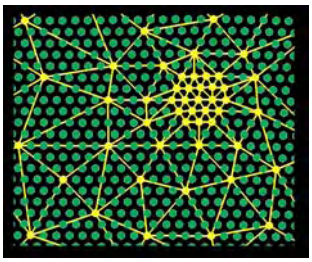

Fig.1. Computational degrees of freedom (yellow atoms) are concentrated near the defect. The positions of the green atoms are linearly interpolated.

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Another main focus has been on extending the capabilities of QC for treating more complex materials. This includes materials with multilattice crystal structures, materials with multiple atomic species, materials where chemistry becomes important, and a new class of organic and non-organic objective structures that constitute a generalization of the idea of a crystal lattice.

Multilattices are crystals that are described as a lattice with a *basis* (a repeating motif of atoms placed at each lattice site). Many technologically important materials from silicon to ferroelectrics and shape-memory alloys have multilattice structures. A common feature of such materials is their tendency to undergo temperature and stress-induced phase transformations. Simulating such materials within QC can be difficult since in some cases the Cauchy-Born kinematics used in continuum regions can fail because the peridocity of the minimizing equilibrium structure cannot be described by the original lattice representation. We have addressed this fundamental shortcoming for the first time by developing a *Cascading Cauchy-Born* kinematics that uses a phonon stability analysis to detect period extensions and adapt the model appropriately. Fig. 2 shows recent results.

To correctly treat chemistry within a multiscale method, a quantum mechanical description of the region of interest is vital. In QC-DFT, the coupling between a density functional theory (DFT) region and classical atomistic regions is achieved by computing a classical estimate for the interaction energy between these regions.
This approach, which is suitable for simple metals, has the advantage that it is very simple to use and yet delivers good accuracy. Several different DFT codes have been tested, including the NWChem package developed at PNNL. Problems such as the effect of hydrogen on dislocations and cracks in aluminum are being explored.

An exciting recent development in materials physics is the discovery by this team that many important organic and non-organic nanostructures adopt so-called *objective structures*. This is a generalization of the idea of a lattice to structures where the atomic environment of any point can be generated from that of its neighbors through an appropriate translation and rotation (recall that translations are only allowed in crystal structures). So far methods for modeling perfect objective structures have been developed, such as objective molecular dynamics. We are now turning to the development of an objective QC.

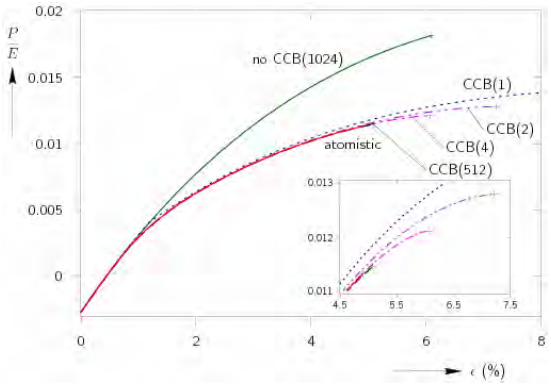

Fig. 1 *Stress versus strain curve for a tension test on a phase transforming material. The standard QC model without Cascading Cauchy-Born (CCB) kinematics fails to capture the correct behavior. CCB models with various levels of refinement converge to the exact result.*

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