Atomistic-to-Continuum Coupling Through Domain Decomposition, Virtual Controls, and Optimization

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ABSTRACT

Atomistic-to-Continuum (AtC) methods are multiphysics models of materials used to simulate atomistic systems on a size scale unreachable on even the largest modern computers. A cornucopia of AtC algorithms have been designed and implemented, but the core feature among them is the decomposition of the computational domain into an atomistic region modeled using an atomistic model such as a Lennard-Jones potential and a continuum region modeled according to some continuum mechanics formulation such as nonlinear elasticity. Though much information can be gleaned from the individual atomistic and continuum models, the mathematical analysis of the errors involved in the coupled approximations are just now beginning to be understood. Such an analysis is vital to both guide the choice of AtC method and optimize its efficiency.

A convenient model problem for comparing the errors of various AtC methods has been simulating a single defect embedded in an infinite crystalline environment in Euclidean space. This allows the error to be generically decomposed into a far-field error resulting from truncating the problem to a finite domain, a coarsening error due to efficiently solving the continuum problem (e.g. using finite elements), and a coupling error arising from coupling the two models.

This work presents the optimization-based AtC algorithm of [1] in the context of a point defect in an infinite lattice and provides error estimates for the three aforementioned errors in two and three dimensions. The method relies on overlapping atomistic and continuum regions with individual atomistic and continuum subproblems. These two problems are coupled together using a virtual control technique developed in [2] to couple advection-diffusion PDEs. A cost functional consisting of the H^1 seminorm of the difference between atomistic and continuum states is minimized subject to the constraints that the atomistic and continuum equilibrium equations hold on each subdomain.

REFERENCES

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