Mathematical Analysis of Atomistic-to-Continuum (AtC) Coupling Methods

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Summary

Atomistic-to-Continuum (AtC) coupling is a critical component in computational materials science and other applications of interest to the DOE Office of Science. Past research in AtC model and algorithm development has been primarily driven by applications and has paid off in the formulation of effective procedures that address specific applications. This previous research has also begun to lead to some degree of generalization. However, much less effort has been directed at the mathematical theory of AtC methods and the formal error, stability, and convergence analysis and uncertainty quantification of the coupling process. The focus of this project is the development of a general mathematical framework that can provide a unified theoretical foundation for the formulation, analysis and implementation of AtC coupling. Our work during the past year considered two approaches. The first investigates the efficacy of using peridynamics as an intermediate scale between continuum and atomistics. A step in this direction is achieved by introducing a notion of peridynamic stress and traction vector. The second approach investigates the interplay between overlapping domain decomposition theory and AtC coupling methods.

Peridynamics (PD) is a microcontinuum theory that employs a nonlocal force model in order to describe long-range material interaction. The force interactions occurring at finite distances are naturally accounted for in PD. Moreover, PD's non-local force model is entirely consistent with those used by atomistic methods, in stark contrast to classical continuum mechanics. Hence, PD can be employed for mesoscopic phenomena that are beyond the realms of classical continuum mechanics and atomistic simulations, e.g. molecular dynamics and density functional theory (DFT). The latter two atomistic techniques are handicapped by the onerous length and time scales associated with simulating mesoscopic materials. This suggests that peridynamics can be applied to space and time scales that are typically beyond the domain of atomistic and classical continuum simulations. In particular, we focus on coupling PDs with classical continuum mechanics.

The equation of motion in the peridynamic model is an integro-differential equation. We derived a notion of a PD stress tensor derived from nonlocal interactions. At any point in the body, this stress tensor is obtained from the forces within PD bonds that geometrically go through the point. The PD equation of motion can be expressed in terms of this stress tensor, and the result is formally identical to the Cauchy equation of motion in the classical model, even though the classical model is a local theory. We also establish that this stress tensor field is unique in a certain function space

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compatible with finite element approximations. In analogy with Cauchy's theorem, we show that the PD traction vector is linear in the normal of an oriented surface. This traction vector can be used as input to a classical continuum mechanics code (say based on finite elements). Our research has resulted in the publication *Force Flux and the Peridynamic Stress Tensor* by Rich Lehoucq, Stewart Silling, accepted for publication in the Journal of Mechanics and Physics of Solids.

We also implemented PD within the public domain massively parallel molecular dynamics (MD) code LAMMPS. This provides MD users the ability to perform continuum mechanical simulations, and AtC multiscale computations.

Our second approach considered overlapping domain decomposition methods, overlapping atomistic and classical continuum mechanical simulations. Because fully atomistic simulations on an entire model domain are computationally infeasible, a common practice is to replace the atomistic model by a continuum model in all regions where the solution is sufficiently smooth. The two models must then be blended in an interface region.

Merging of atomistic and continuum models is fundamentally different from merging continuum models. Because the atomistic model is non-local, one cannot simply truncate it to a subregion; care must be taken to compensate for possible surface effects created by missing bonds. Typically, this means that an atomistic-to-continuum (AtC) coupling method cannot rely solely on transmission conditions at a surface. The main focus of our work is on AtC coupling methods that, in 3 dimensions, blend the two models over a 3-dimensional blending region rather than at a 2-dimensional manifold. A straightforward way to couple atomistic and continuum models is to superimpose the two models in the blending region. Unfortunately, this additive approach leads to unphysical behavior because the resulting effective material strength in the blending region is a superposition of atomistic and continuum strengths. To avoid this duplication, the two models must be "blended" together in such a way that the coupled model has the desired physical response. We state mathematical criteria to quantify such responses by formalizing the notions of patch and consistency tests.

Typically, such models are defined using blending functions that form a partition of unity in the blending region, with solution continuity being enforced via a constraint operator. The constraint may be imposed by: 1) using Lagrange multipliers (in classical or augmented form), or 2) using an AtC space where the constraint is automatically satisfied. The two approaches lead to different AtC operators but are mathematically equivalent.

Our analysis exploits this equivalence by relying on the simpler mathematical structure of the AtC coupling formulation in terms of hybrid spaces. Our research has resulted in one publication *A Force-Based Blending Model for Atomistic-to-Continuum Coupling*, Santiago Badia, Pavel Bochev, Jacob Fish, Max Gunzburger, Rich Lehoucq, M. Nuggehally, Mike Parks, accepted for publication in the International Journal for Multiscale Computational Engineering. This publication considered one variant described by the framework above.

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