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 interplay between domain decomposition theory and AtC coupling methods. The second investigates the efficacy of using peridynamics as an intermediate scale between continuum and atomistics.

One research direction pursued this fiscal year was to relate AtC coupling with domain decomposition (DD) and to leverage the rich mathematical theory for DD. Consider for an example the Finite Element/Atomistic (FEAt) method where the coupled solution is computed by alternating between minimization of atomistic and continuum energy. This process is reminiscent of the basic step in the classical Schwarz alternating method. However, unlike the classical case, the coupled atomistic-continuum problem lacks a global minimization problem. Indeed, the main mathematical difficulty in our analysis stems from the fact that on each subdomain there exists a well-defined atomistic and continuum energy minimization principles, however, these principles cannot be viewed as being restrictions of a single "master" minimization principle valid on the whole domain. This assumption is fundamental in the analysis of conventional overlapping Schwartz methods, but had to be circumvented for the AtC method. Our analysis shows that, similarly to the classical Schwarz method, the AtC scheme converges

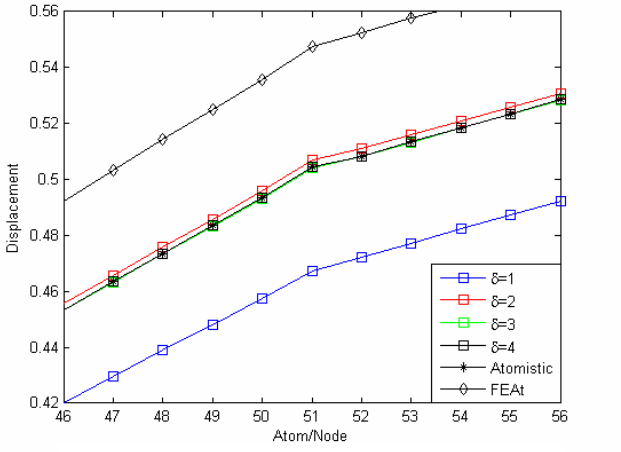

Fig. 1 Dependence of the converged AtC solution on the overlap δ between the atomistic and continuum regions

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in faster when the overlap δ between the atomistic and continuum regions is larger. However, unlike the classical method, the converged AtC solution is also *a function of the amount of overlap;* see Fig. 1. In particular, our analysis and experiments demonstrate that in one dimension, having an overlap of only one atom may not be enough to reproduce the desired solution.

We also considered the peridynamic theory of material deformation and failure as an approach for AtC coupling analysis. The peridynamic theory, introduced by Silling (Sandia National Laboratories 2000), is formulated in terms of integral equations that are based on pair or multibody interactions between particles. The notion of what a particle represents is flexible, permitting a scaling from atomic interactions to continuum elastic behavior between material regions within a body. This is in contrast to existing approaches that seek to synthesize an atomistic approach based on individual non-local force interactions between atoms or molecules with a continuum calculation that deals with bulk quantities that represent the average behavior of millions of atoms or molecules. Hence, peridynamics is potentially well suited for coupling with atomic scale methods, such as molecular dynamics (MD), because of the reliance on non-local force interactions. At the same time, the peridynamic model allows seamless transition to a continuum model, thus enabling a potentially powerful coupling mechanism between vastly different scales.

We invested a significant effort in learning the fundamentals of molecular dynamics from the perspective of numerical analysis. While much literature exists on molecular dynamics, little of this literature concerns itself with accessing the quality of trajectory based phase-space sampling techniques. During Feb. 13-15, Professor Don Estep (collaborative PI) and two graduate students spent two days at Sandia National Laboratories in Albuquerque attending an intensive two day workshop on molecular dynamics prepared by the PI.

A high-point of the fiscal year was a two-day workshop on atomistic-to-continuum (AtC) coupling analysis that was held in Albuquerque, New Mexico. The workshop was sponsored by the Computer Science Research Institute at Sandia National Laboratories and organized by Claude Le Bris (´Ecole Nationale des Ponts et Chauss´ees), Jacob Fish (Rensselaer Polytechnic Institute), and Pavel Bochev, Rich Lehoucq, and Greg Wagner (Sandia National Laboratories). The goal of this workshop was to bring together a group of scientists to understand and quantify the limits in Atomistic-to-Continuum (AtC) coupling and the resulting impact on multiscale simulations. The workshop presented an excellent opportunity for the Sandians to learn about different approaches for AtC coupling and to interact with leading researchers about our own research. Further information is available at http://www.cs.sandia.gov/CSRI/Workshops/2006/AtCCouplingMethods/index.html. An article summarizing the workshop is to be published in a forthcoming issue of the SIAM news.

For further information on this subject contact:

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