Researchers Discuss Atomistic-to-Continuum (AtC) Coupling

Michael L. Parks† and Richard B. Lehoucq†

April 12, 2006

On March 20, 2006, researchers from around the world gathered in Albuquerque, New Mexico, for a two-day workshop on atomistic-to-continuum (AtC) coupling analysis. The workshop was sponsored by the Computer Science Research Institute at Sandia National Laboratories and organized by Claude Le Bris (École Nationale des Ponts et Chaussées), Jacob Fish (Rensselaer Polytechnic Institute), and Pavel Bochev, Rich Lehoucq, and Greg Wagner (Sandia National Laboratories). The goal of the workshop was to understand and quantify the limits in Atomistic-to-Continuum (AtC) coupling and their resulting impact on multiscale simulations.

Many important physical phenomena, such as deformation and failure, are inherently multiscale processes that cannot always be modeled with a traditional finite element analysis. Typically this inability is either because the scale of the domain is small enough that the continuum approximation becomes dubious, or because complex atomistic processes affect macroscopic behavior. In these situations one must resort to an atomistic description to resolve the underlying physics. Unfortunately, fully atomistic simulations of most domains of interest are computationally infeasible, so multiscale modeling methods coupling atomistic and continuum simulations are considered. AtC coupling enables a continuum calculation to be performed over the majority of a domain of interest while limiting the more expensive atomistic simulation to a subset of the domain. Unfortunately, combining atomistic and continuum calculations is challenging because the former is based on individual non-local force interactions between atoms while continuum calculations deal with bulk properties of matter that represent the averaged behavior of huge numbers of atoms. This requires methods to couple across length and time scales spanning many orders of magnitude—from the atomic to the macroscopic.

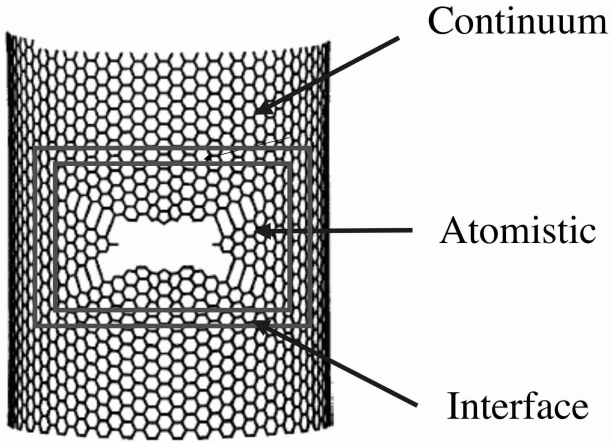

Figure 1: Illustration of AtC carbon nanotube fracture simulation with atomistic domain surrounding failure region and continuum domain elsewhere. The domains are bridged with an interface or "handshake" region. Image courtesy of T. Belytschko [1].

Applications have been a driving force behind the development of AtC coupling methods. For example, an understanding of the failure of carbon nanotubes (CNTs) is needed in order to design CNT-reinforced composites. This has motivated AtC simulations of CNTs in order to model their physical properties, and the effects of defects. In this case a fully atomistic simulation is infeasible, so atomistic representations are used in localized regions where individual atom positions are important and a less expensive continuum representation is used elsewhere, as shown in

†Sandia National Laboratories, Computational Mathematics and Algorithms, P.O. Box 5800, MS 1110, Albuquerque NM 87185 (mlparks@sandia.gov, rblehou@sandia.gov). Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under contract DE-AC04-94-AL85000.

Figure 1. The two simulations are coupled through an interface or "handshake" region. Another important application is the modeling of material failure, which also requires understanding and modeling nanoscale behavior. The material around a crack tip experiences large deformations, and the assumptions of linear elasticity break down in this region. Fracture models based on continuum mechanics theories, such as cohesive surface models, require a priori knowledge about the failure path, whereas atomistics need no such information. In an AtC simulation the region immediately surrounding the crack tip is modeled with atomistics (possibly including quantum mechanical principles) and the remaining region with a finite element model. Coupling of atomistic and continuum simulations provides a computationally efficient mechanism to investigate not only the behavior of crack tips at a fundamental level, but also other phenomena including grain boundaries and dislocations. For overviews of existing methods and techniques, the reader is directed to the surveys by Curtin and Miller (2003) [5], Vvedensky (2004) [12], Fish [8], and an overview of recent mathematical results by Blanc, Le Bris, and Lions (2006) [4].

Recently, the DOE Office of Advanced Scientific Computing Research (ASCR) of the Office of Science solicited proposals for multiscale mathematics research and education. The *Atomic to Macroscopic Mathematics* research effort seeks to develop a deeper understanding of the mathematics of physical phenomena at multiple length and time scales, and how they interact. Further information can be found in the RFP at `www.science.doe.gov/grants/FAPN05-16.html`.

While numerous AtC algorithms have been developed for specific applications, much less effort has been directed at the mathematical theory of AtC methods. A rigorous mechanical formulation and error, stability, convergence analysis, and uncertainty quantification of coupling atomistic and continuum models is lacking. As a result, a mathematical and mechanical framework that can provide a unified theoretical foundation for the formulation, analysis, and implementation of AtC coupling methods is an important open problem that served to focus the AtC workshop.

The workshop featured eight speakers, whose talks addressed several fundamental issues with AtC coupling, including the pros and cons of existing AtC coupling methods, fundamental mechanical distinctions between atomistic and continuum models and their impact upon coupling models, and the physical relations that must hold for any valid coupling method. The workshop provided a forum for individuals to present their research to colleagues in the AtC field and to receive feedback.

The first speaker, Mark Robbins from Johns Hopkins University, discussed how to connect atomic motion to macroscopic behavior. Dealing with both fluid and solid problems, Professor Robbins demonstrated a robust hybrid multiscale method to tie together continuum and atomistic domains across disparate length and time scales. In his framework, atomistic and continuum simulations were coupled through the use of overlap regions in which the continuum region sets boundary conditions for the atomistic region, and the atomistic region sets boundary conditions for the continuum region. Among other examples, Professor Robbins presented highly accurate results for true bidirectional coupling between atomistic and continuum domains for dynamic Couette flow while correctly accounting for mass and heat flux [9].

The next speaker, J. Tinsley Oden of the University of Texas, motivated his talk by telling the audience that the path to error was also the path to truth. (To arrive at the truth we need only quantify the error and remove it!) Professor Oden noted that in any simulation, we describe a physical event by a mathematical model with the goal of calculating some quantity of interest. In general, the actual mathematical model we seek to solve is intractable, so we replace it with a tractable surrogate model. This gives us (almost) the right answer for the surrogate model, but still the wrong answer for the true model. Professor Oden introduced the idea of Goal Oriented Adaptive Modeling [10], a general framework based on an error estimation module that estimates the error between two different models (measured in terms of quantities of interest) and an adaptive algorithm module that automatically selects the models to be used in the various regions of the computational domain. As an example, the specific problem of the analysis of complex multiscale behavior encountered in the nano-manufacture of computer chips was discussed.

Heading the afternoon session was Leonid Berlyand from Penn State, who discussed two separate topics. The first dealt with continuum and discrete models of highly packed particle filled composites. Starting from a continuum PDE model, a discrete network approximation was derived. This model, which can be thought of as a structural discretization rather than

a numerical discretization, provides physical understanding of this problem not readily extractable from the corresponding continuum model. The second topic started with a discrete mass-spring system and developed sufficient conditions on when the network admits a rigorous continuum limit using the method of mesocharacteristics and the discrete Korn's inequality [2]. This result is applicable to non-periodic arrays of particles, of which periodic arrays may be treated as a special case.

The last speaker for the first day was Frédéric Legoll of École Nationale des Ponts et Chaussées, who gave a detailed analysis of a prototypical one-dimensional AtC coupling scheme [3]. Dr. Legoll considered the case of a solid that deforms smoothly in some region but not smoothly in another region, wherein both atomistic and continuum models can be used and must be coupled together. The efficacy of such a technique is dependent on the body force applied to the model. Additional difficulties arise if the interatomic potential model is not convex. Discretizing the continuum region with finite elements resolves some of these issues, essentially regularizing the model.

The second day's first speaker was Ron Miller from Carleton University. His talk opened with a brief overview of the quasicontinuum (QC) method, which was developed for zero temperature problems. He then discussed how QC could be extended to finite temperature simulations through a correction to the QC Hamiltonian. Analogous to the *ghost force correction* used in zero temperature QC, this correction was denoted a *ghost entropy correction*. Even though a quasi-harmonic approximation was used to model the atomic motion, the resulting finite temperature QC formulation was shown in several examples to reproduce the thermal expansion and temperature dependent elastic constants of the underlying atomistic model with only modest error even at high temperatures [6].

Xiantao Li from Penn State spoke on his joint work with Weinan E of Princeton on appropriate boundary conditions for the molecular dynamics simulations of crystalline solids [7]. A desirable MD boundary condition prevents phonon reflection, maintains a correct temperature, and allows coupling with a continuum. An exact reflectionless MD boundary condition can be determined, but this boundary condition is nonlocal in both space and time, and its time-history kernel decays quite slowly. As such, much research has gone into determining less computationally expensive alternatives. Li demonstrated one such alternative, based on a variational approach, that could closely reproduce the exact solution.

The first talk of the the afternoon session was given jointly by Eduard G. Karpov of Northwestern University and Dong Qian of the University of Cincinnati, who discussed the bridging scale approach for AtC coupling. Unlike many other AtC methods that require refining a finite element mesh down to an atomic lattice, bridging scale instead overlays an atomistic domain with a finite element mesh and projects the atomistic solution onto the mesh, avoiding issues associated with extreme refinement of the finite element mesh. The speakers covered general AtC issues within the framework of the bridging scale method, and also introduced the virtual atom cluster (VAC) model [11].

The last presentation of the workshop was a joint talk by Bob Haber and Ph.D. candidate Brent Kraczek of the University of Illinois at Urbana-Champaign on AtC coupling within a spacetime discontinuous Galerkin (SDG) framework. The speakers introduced SDG first in a continuum setting, then in an atomistic setting, and finally discussed how these two could be coupled. The SDG formulation effectively balances energy and momentum between the continuum and atomistic regions, achieving highly accurate numerical results.

The workshop concluded with an open-floor session where current directions and open problems were discussed. In particular, it was observed that model validation will require closer interaction between mathematicians and physical scientists.

Slides from the speakers can be found on the conference website, `www.cs.sandia.gov/CSRI/Workshops/2006/AtCCouplingMethods/`. A special issue of the International Journal for Multiscale Computational Engineering (`www.begellhouse.com/journals/61fd1b191cf7e96f.html`) will publish papers on the workshop theme of AtC coupling analysis. In approximately a year, a second workshop will be organized by J. Tinsley Oden at the University of Texas at Austin.

The authors acknowledge helpful comments from Pavel Bochev, J. Fish.

M. L. Parks is a postdoctoral employee at Sandia National Laboratories, supervised by R. B. Lehoucq and P. B. Bochev. His webpage (`www.cs.sandia.gov/~mlparks/`) details his work and research interests, which include multiscale analysis, iterative methods, domain decomposition, and numerical lin-

ear algebra. R. B. Lehoucq is a Member of the Technical Staff at Sandia National Laboratories.

References

[1] T. Belytschko, S. P. Xiao, G. C. Schatz, and R. S. Ruoff, *Atomistic simulations of nanotube fracture*, Phys. Rev. B, 65 (2002).

[2] M. Berezhnyy and L. Berlyand, *Continuum limit for three-dimensional mass-spring networks and discrete Korn's inequality*, J. Mech. Phys. Solids, 54 (2006), pp. 635–669.

[3] X. Blanc, C. L. Bris, and F. Legoll, *Analysis of a prototypical multiscale method coupling atomistic and continuum mechanics*, Math. Model. Num. Anal., 39 (2005), pp. 797–826.

[4] X. Blanc, C. L. Bris, and P. L. Lions, *Atomistic to continuum limits for computational materials science*. Submitted. Available at `www.ann.jussieu.fr/publications/2005/R05048.pdf`, 2006.

[5] W. Curtin and R. Miller, *Atomistic/continuum coupling methods in multi-scale materials modeling*, Modeling and Simulation in Materials Science and Engineering, 11 (2003), pp. R33–R68.

[6] L. Dupuy, E. Tadmor, R. Miller, and R. Phillips, *Finite temperature quasicontinuum: Molecular dynamics simulations without all the atoms*, Phys. Rev. Lett., 95 (2005), p. 060202.

[7] W. E and X. Li, *Boundary conditions for molecular dynamics simulations of solids at low temperature*, Comm. Com. Phys., 1 (2006), pp. 136–176.

[8] J. Fish, *Bridging the scales in nano engineering and science*, J. Nanopart. Res., (2006). In print.

[9] X. B. Nie, S. Y. Chen, W. N. E, and M. O. Robbins, *A continuum and molecular dynamics hybrid method for micro- and nano-fluid flow*, J. Fluid Mech., 500 (2004), pp. 55–64.

[10] J. T. Oden and K. Vemaganti, *Estimation of local modeling error and goal-oriented adaptive modeling of heterogeneous materials; part I : Error estimates and adaptive algorithms*, J. Comp. Physics, 164 (2000), pp. 22–47.

[11] D. Qian and R. Gondhalekar, *A virtual atom cluster approach to the mechanics of nanostructures*, Internat. J. Multiscale Comp. Eng., 2 (2004), pp. 277–289.

[12] D. D. Vvedensky, *Multiscale modelling of nanostructures*, J. Phys. Condens. Matter, 16 (2004), pp. R1537–R1576.