SAND2007-3498C

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

Colorado State University
Donald Estep, PI

Florida State University
Max Gunzburger, PI

Rennselaer Polytechnic Institute
Jacob Fish, PI
Mark Shephard, Co-PI

Sandia National Laboratories
Richard B. Lehoucq, PI
Pavel Bochev, Co-PI

May 16, 2007

Rich Lehoucq, Mike Parks

Sandia National Labs, Albuquerque

Computational Math & Algorithms

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Sandia National Laboratories

Our Multiscale Research

- Litany of phenomenological methods—our goal is to understand existing methods
  - Little rigorous analysis of schemes exists
  - Lack of a rational mechanical foundation
- Goal: a numerical analysis of AtC coupling methods
- ***Our presentation overviews our group's work***

Proposal Cover Sheet
DOE Program Announcement LAB 05-16

Collaborative Proposal:
A Mathematical Analysis of Atomistic-to-Continuum (AtC) Coupling Methods

U.S. DEPARTMENT OF ENERGY

The Office of Science is now using The Department of Energy e-Center Industry Interactive Procurement System (IIPS) for the electronic submission of applications. Please reference IIPS number DE-FG01-05ER05-16

Office of Science
Notice DE-FG01-05ER05-16

Multiscale Mathematics Research and Education

Department of Energy

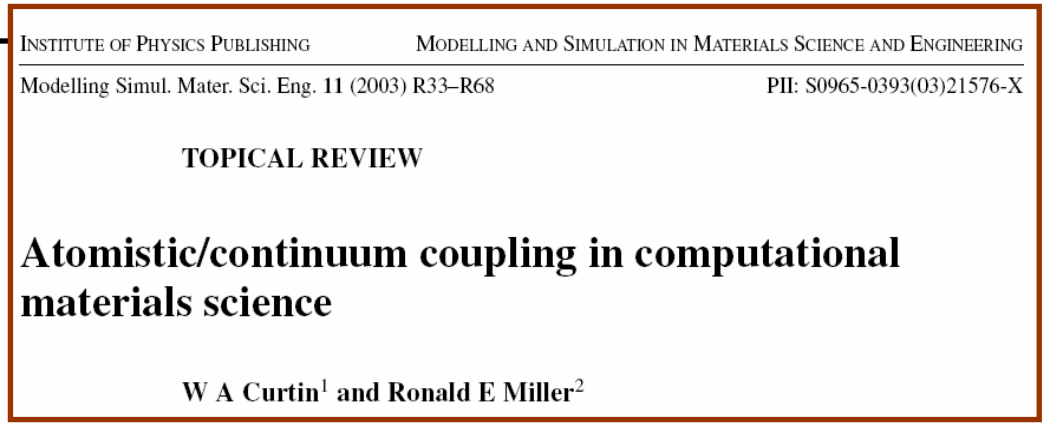
Office of Science Financial Assistance Program Notice DE-FG01-05ER05-16: Multiscale Mathematics Research and Education

AGENCY: U.S. Department of Energy

Sandia National Laboratories

Why AtC coupling?

- Couple atomistic and continuum models
  - Augment continuum model with microscale information
  - Extend atomistic methods
- Enables mesoscopic capability
  - Failure modeling
  - Microstructure (defects, dislocations)
  - Nanostructures
- Useful to couple A and C when a material model is not available for C or A



INSTITUTE OF PHYSICS PUBLISHING MODELLING AND SIMULATION IN MATERIALS SCIENCE AND ENGINEERING

Modelling Simul. Mater. Sci. Eng. **11** (2003) R33–R68 PII: S0965-0393(03)21576-X

TOPICAL REVIEW

Atomistic/continuum coupling in computational materials science

W A Curtin[1] and Ronald E Miller[2]

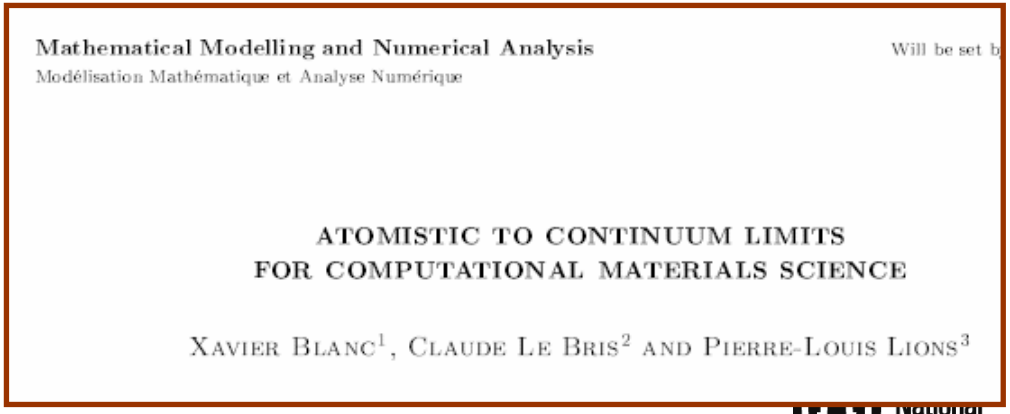
INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS: CONDENSED MATTER

J. Phys.: Condens. Matter **16** (2004) R1537–R1576 PII: S0953-8984(04)55699-0

TOPICAL REVIEW

Multiscale modelling of nanostructures

Dimitri D Vvedensky



Mathematical Modelling and Numerical Analysis Will be set b

Modélisation Mathématique et Analyse Numérique

ATOMISTIC TO CONTINUUM LIMITS
FOR COMPUTATIONAL MATERIALS SCIENCE

XAVIER BLANC[1], CLAUDE LE BRIS[2] AND PIERRE-LOUIS LIONS[3]

National Laboratories

Two Types of AtC

- Zero temperature (quasi-static)
  - Couple the equilibrium equations of molecular statics and continuum mechanics in space

$$0 = -\nabla_{r_\alpha}(r_1, \cdots, r_n) + f_\alpha^e$$

$$0 = \nabla \bullet \sigma + b$$

- Finite temperature (dynamics)
  - Couple equations of molecular dynamics (MD) and continuum mechanics in space and *time*

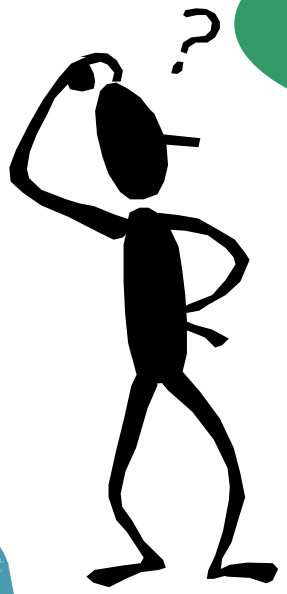
$$m_\alpha a_\alpha = -\nabla_{r_\alpha}(r_1, \cdots, r_n) + f_\alpha^e$$

$$\rho \ddot{u}(x) = \nabla \bullet \sigma + b$$

Sandia National Laboratories

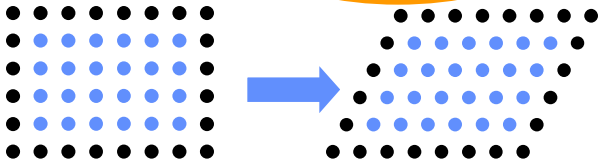
AtC Coupling Frontier

Ghost Forces



Consistency

Cauchy-Born



Exact Solution

Newton's Laws

Convergence

Patch Test

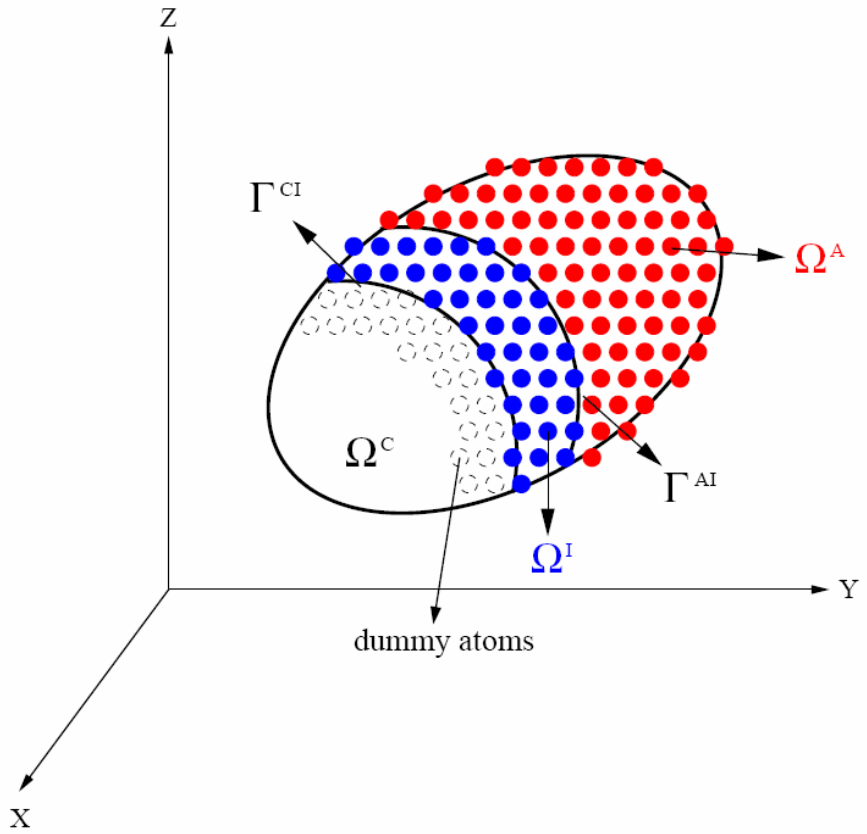
Stability

Classical, continuum, statistical mechanics

Sandia National Laboratories

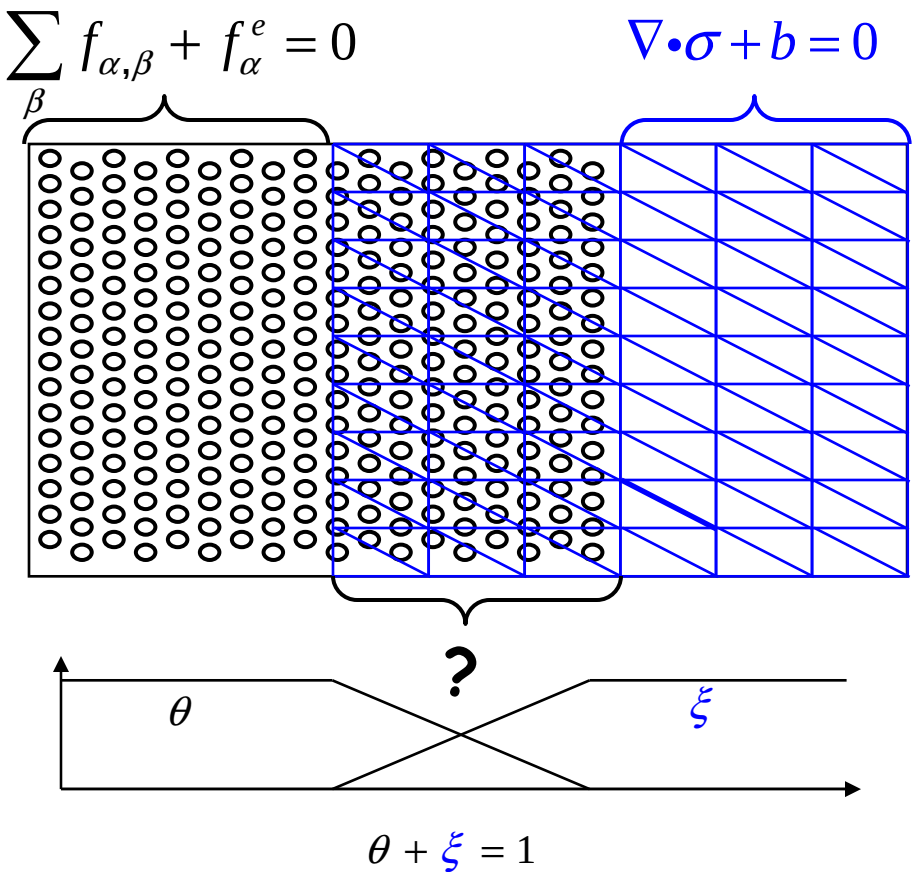
Blending Atomistic and Continuum Models

- AtC coupling as an overlapping domain decomposition method
- Take a cue from the Arlequin method, Ben Dhia IJNME 1998
  - Couple continuum models over a subdomain (not an interface)
  - Oden et al (this morning)
- Bridging Domain Method, Belytschko, Xiao, IJMCE 2004
  - AtC coupling using energy functionals
- Quasicontinuum method (Shenoy, Miller, Tadmor, Rodney, Phillips, Ortiz, 1999) is a special case, i.e. when subdomain is limited to an interface



Sandia National Laboratories

AtC blending



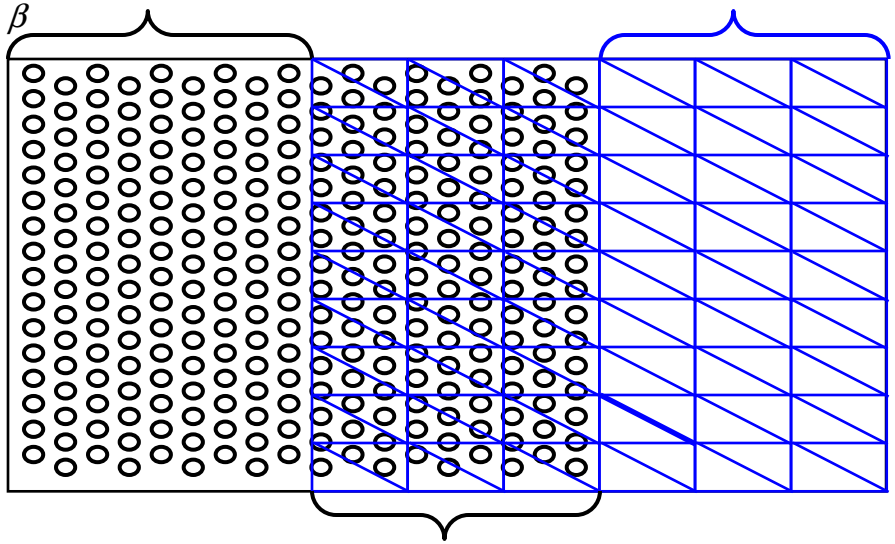
- Individual balance of A and C forces
- Assume A and C both valid on the overlapping subdomain
- How to blend?
- Assume a balance of blended forces in the overlapping subdomain

$$\sum_{\beta} \theta(\boldsymbol{f}_{\alpha,\beta} + \boldsymbol{f}_{\alpha}^{\boldsymbol{e}}) + \nabla \bullet (\xi\sigma) + \xi \boldsymbol{b} = 0$$

Sandia National Laboratories

AtC blending and constraining

$$\sum_{\beta} f_{\alpha,\beta} + f^{e}_{\alpha} = 0 \qquad \nabla \bullet \sigma + b_c = 0$$



$$\sum_{\beta} \theta(\mathbf{f}_{\alpha,\beta} + \mathbf{f}^{e}_{\alpha}) + \nabla \bullet (\xi\sigma) + \xi \mathbf{b}_c = 0$$

- Constrain particle displacements in blend region, say $\mathbf{u}_\alpha = \mathbf{u}^h(\mathbf{x}_\alpha)$, to remove redundancy in the blend region
- Result is a nonlinear system (coupled equilibrium equation)
- Allows computation of residual for the blended model

Sandia National Laboratories

Force-based blending for AtC coupling

- 3D AtC coupling: Aluminum EAM interatomic potential and linear elastic FEM
- Consider microstructure
- Patch test (reproduce homogenous deformation field)
- Careful mechanical consideration of blending A and C forces in 1D
- Meticulous patch test and consistency tests

Concurrent AtC coupling based on a blend of the continuum stress and the atomistic force

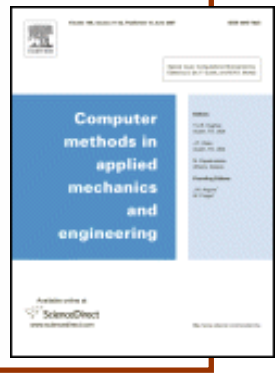
Jacob Fish [a], Mohan A. Nuggehally[b], Mark S. Shephard[c], Catalin R. Picu[d], Santiago Badia [e], Michael Parks [f] and Max Gunzburger [g]

Scientific Computation Research Center
Rensselaer Polytechnic Institute 110 8th St.
Troy NY 12180
[a]fishj@rpi.edu [b]nuggehal@scorec.rpi.edu
[c]shephard@scorec.rpi.edu [d]cpicu@scorec.rpi.edu

Computational Mathematics and Algorithms, MS-1320
Sandia National Laboratories
Albuquerque NM 87185-1320
[e]sibadia@sandia.gov [f]mlparks@sandia.gov

School of Computational Science
Florida State University
Tallahassee FL 32306-4120

Submitted to



A Force-Based Blending Model for Atomistic-to-Continuum Coupling

S. Badia,*† P. Bochev,* J. Fish,‡ M. Gunzburger,§ R. Lehoucq,* M. Nuggehally,‡ M. L. Parks*

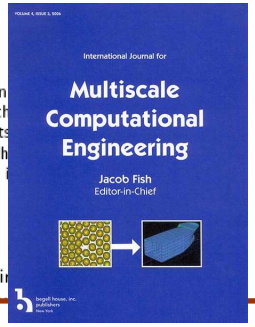
Submitted to

Abstract

A method for coupling atomistic and continuum models across a subdomain presented. Coupling is effected through a force-based blending model. The meth for the the atomistic and continuum contributions to the force balance at points Simple patch tests and computational experiments are used to study the meth in one dimension. A discussion of implementation issues in higher dimensions

1 Introduction

The need to couple atomistic and continuum models arises for two reasons. Fi



Sandia National Laboratories

Abstract AtC Blending Framework

- Canonical form for all AtC blended models

$$A^a_\theta(\psi,\varphi)+A^c_\xi(u,v)=0 \quad \forall v \in R^c_0, \varphi \in R^a_0$$

$$C(u,\psi)=0$$

- For blended atomistic and continuum operators, can blend either balance equations or test functions (four choices)
- We investigate
  - Well-defined notions of AtC consistency and a patch test
  - Ghost-forces
  - Stability, solvability

ON ATOMISTIC-TO-CONTINUUM (ATC) COUPLING BY BLENDING

SANTIAGO BADIA , MICHAEL PARKS , PAVEL BOCHEV , MAX GUNZBURGER , AND RICHARD LEHOUCQ

Abstract. This paper studies coupling of atomistic and continuum problems by using a blending model on an interface region. The continuity of the atomistic and continuum solutions is imposed by a constraint operator that can be enforced using Lagrange multipliers or hybrid atomistic-to-continuum spaces. We develop a mathematical framework for such AtC coupling methods that facilitates their analysis, clarifies the origin of ghost forces and formalizes the notion of a patch test. The framework is applied to study consistency and stability of four representative AtC methods, . Theoretical findings are supported by a series of numerical experiments with the AtC methods.

1. **Motivation.** Fully atomistic simulation on an entire model domain is computationally infeasible for many applications of interest. In such cases, 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 tied together in an interface region, using a suitable "continuity" condition for the atomistic and contin

Sandia National Laboratories

Abstract AtC Blending Framework Summary

Method	Atomistic blend	Continuum blend	Newton's 3rd law	Consistency
I	Test functions	Weak Form	No	No
II	Weak Form	Weak Form	YES	No
III	Test Functions	Test Functions	No	YES
IV	Weak Form	Test Functions	No	No

No method simultaneously satisfies Newton's third law and consistency!

Why?

Incompatibility of force models

Sandia National Laboratories

Why persist with AtC blending?

- Molecular and Classical continuum mechanics use *non-local* and *local* force models, respectively
- AtC blending is of interest because
  - Material models are understood
  - Leverage significant software investment in A and C
    - M. Shephard (RPI) is developing component software to enable AtC coupling of FEM and MD software (e.g. LAMMPS)
    - J. Fish (RPI) considering how to build in MD into the commercial FE code ABAQUS
- ***Goal of our numerical analysis:*** to what extent can the local/nonlocal incompatibility be mitigated to compute quantities of interest?

Sandia National Laboratories

Two Types of AtC

- Zero temperature (quasi-static)
  - Couple the equilibrium equations of molecular statics and continuum mechanics in space

$$0 = -\nabla_{r_\alpha}(r_1, \cdots, r_n) + f_\alpha^e$$

$$0 = \nabla \bullet \sigma + b$$

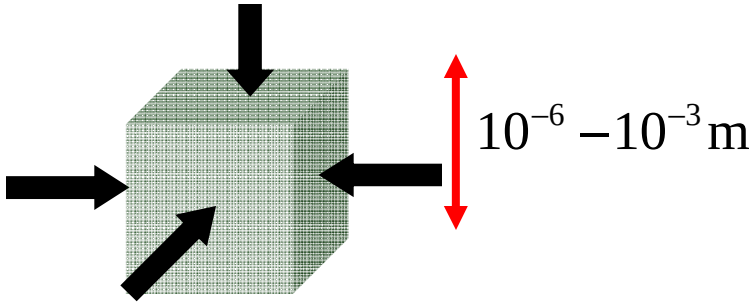
- Finite temperature (dynamics)
  - Couple equations of molecular dynamics (MD) and continuum mechanics in space and *time*

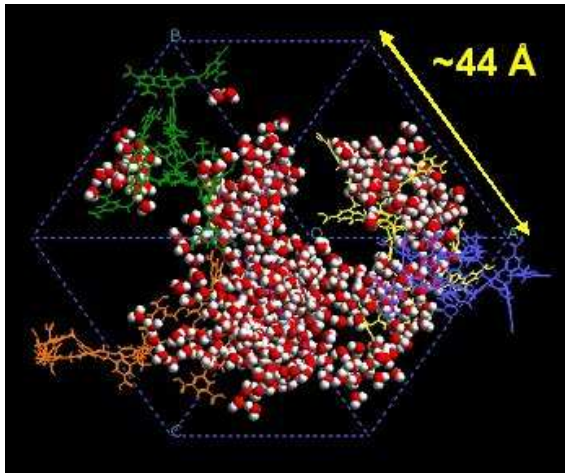
$$m_\alpha a_\alpha = -\nabla_{r_\alpha}(r_1, \cdots, r_n) + f_\alpha^e$$

$$\rho \ddot{u}(x) = \nabla \bullet \sigma + b$$

AtC coupling challenges

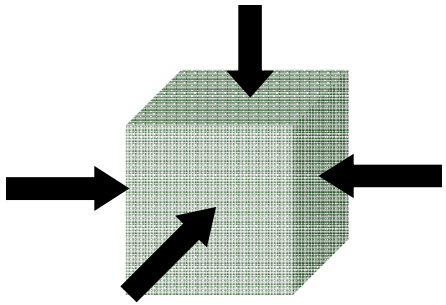
- Classical continuum mechanics assumes
  - Local force model
  - gradient of displacement (perhaps in a weak sense)
  - extremely small wavelengths are not resolved, incorrect dispersion relationships
- Atomistics, or molecular mechanics, assumes
  - non-local force model
  - gradients not assumed
  - non-linear dispersion relationships, small wavelength behavior critical
  - stress is typically a derived quantity and represents a challenge for interatomic potentials of interest
- **Recall, the incompatibility of force models leads to difficulties**





Sandia National Laboratories

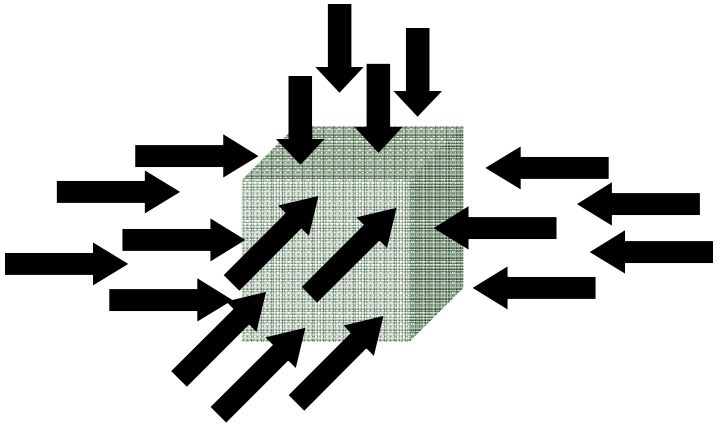
Local and non-local models of force at the continuum level



Classical model (Cauchy): Exterior of cube imparts force to the interior via the surface S

$$\int \mathbf{t}(x,\mathbf{n})dS$$

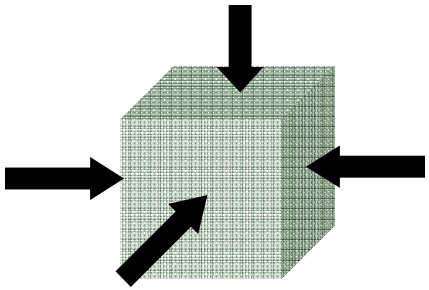
Force is **local** because the postulate is that the force between the interior and exterior can be confined to the surface



Non-local model: Exterior of cube imparts force to the interior—***not just at the surface***

Sandia National Laboratories

Local force model and Cauchy equation of motion (EOM)



$$\boldsymbol{\sigma}(\mathbf{x}) = g(\nabla \mathbf{u})$$

$$\int \mathbf{t}(\mathbf{x},\mathbf{n})dS = \int \boldsymbol{\sigma}(\mathbf{x})\mathbf{n}dS$$

$$= \int \nabla \cdot \boldsymbol{\sigma}(\mathbf{x})dV$$

$$= \int \mathbf{b}dV + \int m\mathbf{a}dV$$

- Cauchy equation of motion assumes
  - gradients of displacement
  - local force model
- Any discretization (FEM, XFEM, SPH, MPM, EFG) that purports to be compatible must assume
  - gradients of displacements
  - local force model
- Of course, you can introduce non-locality at the discrete level
  - But, then, you've at best, a tenuous connection to the mechanical equation—maybe an issue (certainly verification is challenging)
- Of course, why is a non-local model of force of interest?

Sandia National Laboratories

Non-locality does matter

PRL 98, 195504 (2007) PHYSICAL REVIEW LETTERS week ending 11 MAY 2007

Length Scales at which Classical Elasticity Breaks Down for Various Materials

R. Maranganti and P. Sharma*

Department of Mechanical Engineering, University of Houston, Houston, Texas 77204 and Department of Physics, University of Houston, Houston, Texas 77204, USA

(Received 7 February 2007; published 9 May 2007; corrected 11 May 2007)

At what characteristic length scale does classical continuum elasticity cease to accurately describe small deformation mechanical behavior? The two dominant physical mechanisms that lead to size dependency of elastic behavior at the nanoscale are surface energy effects and nonlocal interactions. The latter arises due to the discrete structure of matter and the fluctuations in the interatomic forces that are smeared out within the phenomenological elastic modulus at coarser sizes. While surface energy effects have been well characterized in the literature, little is known about the length scales at which nonlocal effects manifest for different materials. Using a combination of empirical molecular dynamics and lattice dynamics (empirical and *ab initio*), we provide estimates of nonlocal elasticity length scales for various classes of materials: semiconductors, metals, amorphous solids, and polymers.

- Investigates at what length scale the local force assumption of classical elasticity breaks down for various materials
- Occurs at order 100 Å—amorphous materials largest
- Two orders of magnitude larger than length scale of MD—can we use a non-local continuum theory?

Sandia National Laboratories

Peridynamics (PD), Silling 2000

- PD equation of motion (EOM)

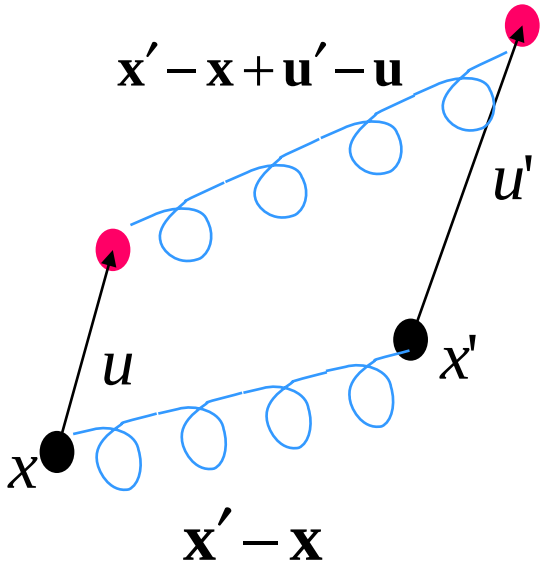
$$\rho\ddot{\mathbf{u}} = \int_R f(\mathbf{u}' - \mathbf{u}, \mathbf{x}' - \mathbf{x}) dV' + \mathbf{b}$$

$$\mathbf{u} = \mathbf{u}(\mathbf{x}, t)$$

$$\mathbf{u}' = \mathbf{u}(\mathbf{x}', t)$$

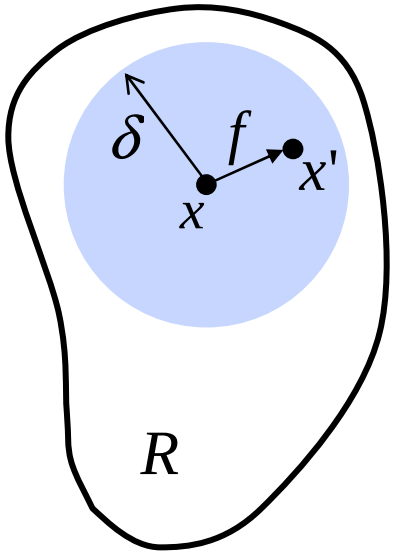
$$\mathbf{b} = \mathbf{b}(\mathbf{x}, t)$$

- $f(\cdot,\cdot)$ is the force density per unit volume that x' exerts on *x*, given
  - relative position x'- x in the reference configuration
  - relative displacement u'-u
- $f(\cdot,\cdot)$ is a pairwise force function



Properties of peridynamic (PD) force functions

$$\int_R f(\mathbf{u}' - \mathbf{u}, \mathbf{x}' - \mathbf{x}) dV'$$



- material-specific behavior is contained in $f(\cdot,\cdot)$
  - and is a function of displacement
- Convenient to assume $f(\cdot,\cdot)$ vanishes outside some horizon $\delta > 0$
- No use of strain—the gradient of displacement is not needed—a "rough" displacement is possible

PD equation of motion

Cauchy equation of motion

$$\rho\ddot{\mathbf{u}} = \nabla\bullet\boldsymbol{\sigma}(\mathbf{x}) + \mathbf{b}$$

$$\boldsymbol{\sigma} = g(\nabla\mathbf{u})$$

$$\rho\ddot{\mathbf{u}} = \int_{\Omega} f(\mathbf{u}'-\mathbf{u}, \mathbf{x}'-\mathbf{x})dV' + \mathbf{b}$$

$$\rho\ddot{\mathbf{u}} = \nabla\bullet\mathbf{v}(\mathbf{x}) + \mathbf{b}$$

Well posed traction can be handed over to classical continuum mechanics (FEM) so that PD to FEM coupling is enabled

Force Flux and the Peridynamic Stress Tensor

R. B. Lehoucq [a,1]

[a] *Computational Mathematics and Algorithms, Sandia National Laboratories, P.O. Box 5800, MS 1320, Albuquerque, NM 87185*

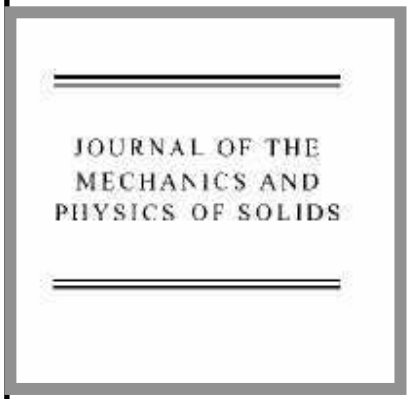
S. A. Silling [b,1]

[b] *Multiscale Dynamic Materials Modeling, Sandia National Laboratories, P.O. Box 5800, MS 1322, Albuquerque, NM 87185*

Abstract

The peridynamic model is a framework for continuum mechanics based on the idea that pairs of particles exert forces on each other across a finite distance. The equation of motion in the peridynamic model is an integro-differential equation. In this paper, a notion of a peridynamic stress tensor derived from nonlocal interactions

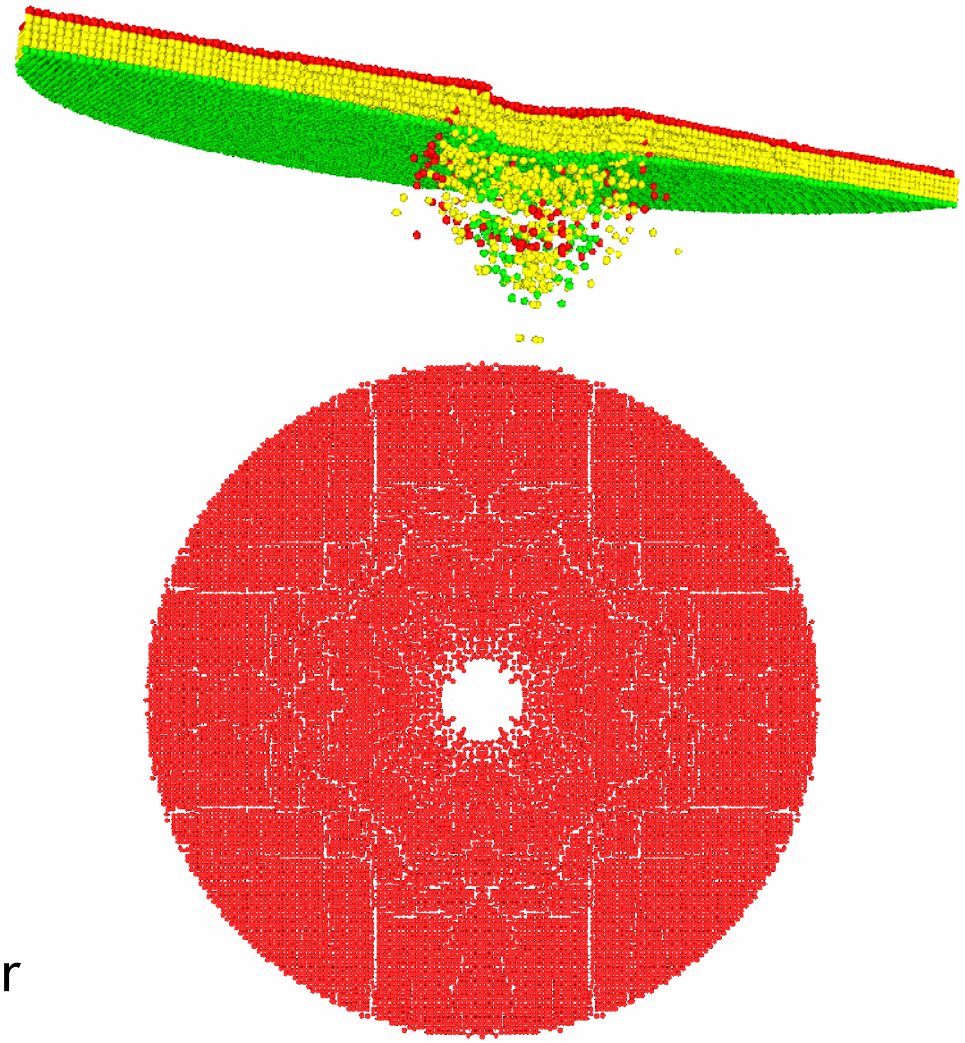
Submitted to



Sandia National Laboratories

PD implementation within LAMMPS

- LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) open source C++ software for MD
- Leverage LAMMPS portability to DOE hardware
- Provide MD users a computational microcontinuum mechanics capability
- Provide PD users the ability to use interatomic potentials
- Lehoucq, Parks, Plimpton, Sandia tech report
- Recall that Shephard (RPI) is developing component software for coupling FEM and MD software (LAMMPS)

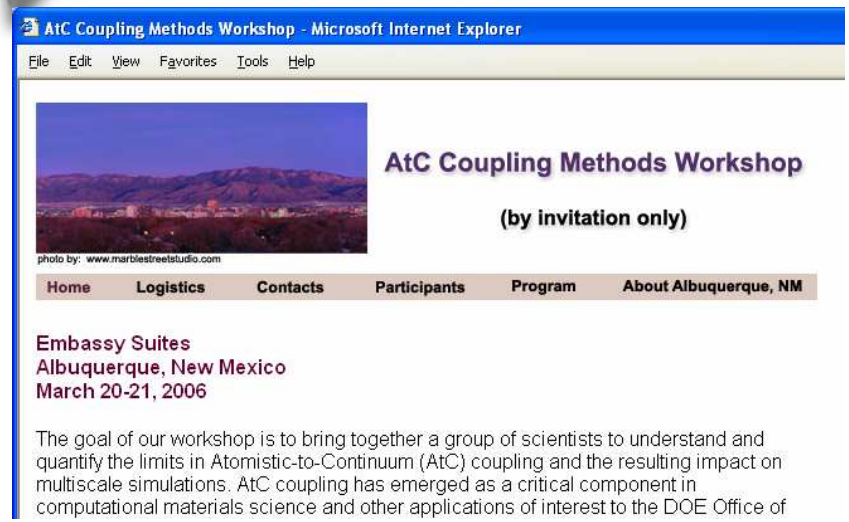


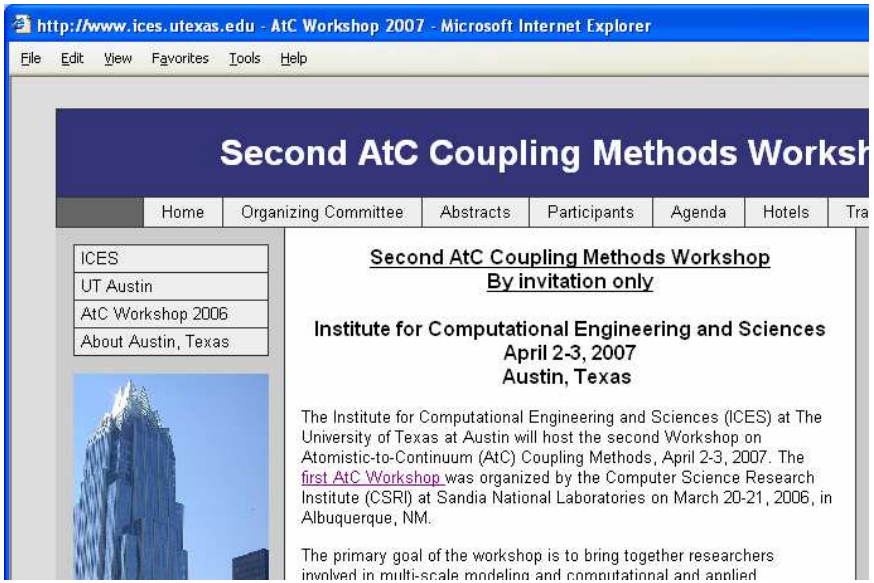
Sandia National Laboratories

Ongoing Work

- Extend blended AtC math framework from a balance of forces to an energy based formulation (Badia, Bochev, Estep, Gunzburger, Parks, Lehoucq)
- Adaptive model selection and error estimation procedure for blended AtC coupling (Estep, Fish, Gunzburger, Shephard)
- Explore relationship between MD and PD; provide a statistical mechanical foundation for PD (Lehoucq, Parks, Silling)
- Relationship between Fish's Generalized mathematical homogenization (GMH) and peridynamics (Lehoucq, Parks, Silling) for finite temperature MD
- Role of constitutive relationships between classical continuum mechanics and peridynamics (Bochev, Lehoucq, Parks)

AtC workshops





- Two AtC workshops—bring together small group of folks
  - SNL 2006
  - UT Austin 2007
  - UMN 2008 or FSU 2008?
- Google on "AtC coupling"
- E., Gunzburger, Luskin, Lehoucq are co-organizers of the 4th *International Multiscale Materials Conference (FSU 10/08)*, feature an extensive (2-3 days) minisymposium on mathematics & AtC coupling

Sandia National Laboratories