CNA Workshop on Macroscopic
Modeling of Materials with Fine Structure

Center for Nonlinear Analysis
Carnegie Mellon University
Pittsburgh, PA

May 26 - 28, 2011

Main Talks			
	Thursday	**Friday**	**Saturday**
Time	**May 26**	**May 27**	**May 28**
8:30-9:00	Continental Breakfast	Continental Breakfast	Continental Breakfast
9:00-10:15	Stewart Silling	Mitchell Luskin	Tony Lelievre
10:15-11:30	Max Gunzberger	Christoph Ortner	Chun Liu
11:30-1:30	Lunch	Lunch	Adjourn
1:30 - 2:45	Florian Theil	Antonio DeSimone	
3:00 - 4:00	CT (1a,b)	CT (3a,b)	
4:00 - 4:20	Coffee Break	Coffee Break	
4:20 - 5:40	CT (2a,b)	CT (4a,b)	

Contributed Talks				
Time	**Thursday, May 26**		**Friday, May 27**	
	CT (1a)	**CT (1b)**	**CT (3a)**	**CT (3b)**
3:00 -3:20	P. Cesana	M. Elsey	M. Chermisi	K. Bojar
3:20-3:40	M. Dai	M. Emelianenko	E. Esenturk	M. Hegg
3:40-4:00	E. Gartland	Y. Epshteyn	L. Wang	M. Veneroni
4:00-4:20	Coffee Break	Coffee Break	Coffee Break	Coffee Break
	CT (2a)	**CT(2b)**	**CT (4a)**	**CT (4b)**
4:20-4:40	J. Marshall	C. Caginalp	M. Renger	G. Simpson
4:40-5:00	T. Mengesha	L. Tan	M. Bocea	X. Wang
5:00-5:20	P. Seleson	D. Zorica	B. Muite	J. Zhang
5:20-5:40	K. Zhou		Y. Sengul	A. Aghaei

Contributed talks sessions (a) will be held in Wean 7218.
Contributed talks sessions (b) will be held in Wean 8220.

There will be a reception Thursday, May 26 from 6:30 PM - 8:00 PM in Schatz Dining Room, located on the second floor of the University Center.

This workshop is sponsored by the Department of Mathematical Sciences at Carnegie Mellon University and the National Science Foundation.

MAIN SPEAKERS

Thursday, May 26
9:00-10:15

Peridynamics and Coarse Graining

Stewart A. Silling
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Abstract: The peridynamic theory is an extension of traditional solid mechanics that treats discontinuous media, including the evolution of discontinuities due to fracture, on the same mathematical basis as classically smooth media. A recent advance in the linearized peridynamic theory permits the reduction of the number of degrees of freedom modeled within a body. Under equilibrium conditions, this coarse graining method exactly reproduces the internal forces on the coarsened degrees of freedom, including the effect of the omitted material that is no longer explicitly modeled. The method applies to heterogeneous as well as homogeneous media and accounts for defects in the material. The coarse graining procedure can be repeated over and over, resulting in a hierarchically coarsened description that, at each stage, continues to reproduce the exact internal forces present in the original, detailed model. Each coarsening step results in reduced computational cost.

This talk will cover the basics of the peridynamic theory. Then the new coarse graining method will be discussed, with computational examples. It will be demonstrated that the method produces accurate effective properties of a composite material.

Thursday, May 26
10:15-11:30

A nonlocal Vector Calculus and the Analysis and Approximation of Nonlocal Models for Diffusion and Mechanics

Max Gunzburger
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Abstract: We study nonlocal models for diffusion and mechanics, including the nonlocal, spatial derivative free peridynamics model for solid mechanics. Our focus is on the analysis of well posedness and on finite element methods. Both rely on a vector calculus we have developed for nonlocal operators that mimics the classical differential vector calculus. Included are the definitions of nonlocal divergence, gradient, and curl operators and the derivation of nonlocal integral theorems and identities. The nonlocal calculus is then applied to nonlocal diffusion and mechanics problems; in particular, strong and weak formulations of these problems are considered and analyzed, showing, for example, that unlike elliptic partial differential equations, these problems do not necessary result in the smoothing of data. Finally, we briefly consider finite element methods for nonlocal problems, focusing on solutions containing jump discontinuities; in this setting, nonlocal models can lead to optimally accurate approximations.

Thursday, May 26
1:30-2:45

Crystallization in Three Dimensions: The FCC Case

Florian Theil
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Abstract: We study the asymptotic behaviour of minimizers of atomistic pair interaction systems of Lennard-Jones type in the limit where the number of particles tends to infinity. For a large class of pair interaction potential it can be shown rigorously that the minimizers converge to a rigid fcc lattice. Novel applications of discrete geometry and rigidity estimates are key ingredients of the proof.

Thursday, May 26
Contributed Talks sessions (1a,1b) 3:00-4:00

Thursday, May 26
4:00-4:20 Coffee Break

Thursday, May 26
Contributed Talks sessions (2a,2b) 4:20-5:40

Friday, May 27
9:00-10:15

Energy-Based Blended Quasicontinuum Approximations

Mitchell Luskin
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Abstract: The development of patch test consistent quasicontinuum energies for multi-dimensional crystalline solids modeled by many-body potentials remains a challenge. The original quasicontinuum energy (QCE) has been implemented for many-body potentials in two and three space dimensions, but it is not patch test consistent. We propose that by blending the atomistic and corresponding Cauchy-Born continuum models of QCE in an interfacial region with thickness of a small number of blended atoms, a general quasicontinuum energy (BQCE) can be developed with the potential to significantly improve the accuracy of QCE near lattice stabilities such as dislocation formation and motion.

We give an error analysis of the blended quasicontinuum energy (BQCE) for a periodic one-dimensional chain of atoms with next-nearest neighbor interactions which allows the blending function to be optimized for an improved convergence rate. We show that the $\ell 2$ strain error for the non-blended QCE energy (QCE), which has low order $\mathrm{O}(\varepsilon^{1/2})$ where ε is the scaled atomistic length scale, can be reduced by a factor of $k^{3/2}$ where k is the number of atoms in the blending region. The QCE energy has been further shown to suffer from a O(1) error in the critical strain at which the lattice loses stability. We prove that the error in the critical strain of BQCE can be reduced by a factor of $k2$ where k is the number of atoms in the blended interface region, thus demonstrating that the BQCE energy has the potential to give an accurate approximation of the deformation near lattice instabilities such as crack growth. Joint with Brian Van Koten.

Friday, May 27
10:15-11:30

The Role of the Patch Test in Atomistic-to-Continuum Coupling Methods

Christoph Ortner
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Abstract: Low energy equilibria of crystalline materials are typically characterized by localized defects that interact with their environment through long-range elastic fields. By coupling atomistic models of the defects with continuum models for the elastic far field one can, in principle, obtain models with near-atomistic accuracy at significantly reduced computational cost. Several pitfalls need to be overcome to construct a reliable coupling mechanism. Possibly the most widely discussed among these are the so-called ghost forces that typically arise in energy-based A2C coupling mechanisms.

In this talk I will first describe the construction of energy-based A2C coupling methods, how ghost forces arise, and present some ideas how to avoid them. I will then explain the resulting modelling errors due to different types of interface treatment. I will give partial answers to the fundamental theoretical question whether absence of ghost forces automatically implies "high accuracy of the coupling scheme.

Friday, May 27
1:30-2:45

Microstructures in Nematic Elastomers: Modeling, Analysis, and Numerical Simulation

Antonio DeSimone
Scuola Internazionale Superiore di Studi Avanzati
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Abstract: In this talk, we will review the recent progress on the modelling of martensitic-like microstructures in nematic elastomers, and on coarse-grained models for their effective mechanical response based on the use of the quasi-convex envelope of the stored energy density.

Friday, May 27
Contributed Talks sessions (3a,3b), 3:00-4:00

Friday, May 27
Coffee Break
4:00-4:20

Friday, May 27
Contributed Talks sessions (4a,4b), 4:20-5:40

Saturday, May 28
9:00-10:15

A Mathematical Viewpoint on Multiscale Models for Polymeric Fluids

Tony Lelièvre
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Abstract: We will first present some multiscale (or micro-macro) models which have been introduced to describe the behaviour of polymerics fluids. These models rely on the coupling of classical momentum and mass conservation equations at the macroscopic level, with kinetic equations to model the evolution of the polymers within the fluid, that yield the stress through ensemble averages. After a short discussion of the modelling approach, we will present two mathematical aspects: (i) the long-time behaviour for such models and the derivation of free-energy dissipative finite element schemes and (ii) some numerical approaches to obtained closed evolution on the stress, starting from a micro-macro model.

Saturday, May 28
10:15-11:30

Electrostatics and Ion Transport for Nondiluted Ionic Fluids

Chun Liu
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Abstract: In this paper, we will present some recent analytical results related to modeling ionic fluids. In particular, we will focus on the phenomena that are relevant to the ion distribution and transport in proteins and other biological environments.

CONTRIBUTED TALKS
Abstracts: http://www.math.cmu.edu/cna/macro2011/sched.html
Thursday, May 26

Session 1a, Wean 7218
3:00-3:20

Relaxation Results for Nematic Elastomers

Pierluigi Cesana
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Session 1b, Wean 8220
3:00-3:20

Extending DFDGM to Motion by Weighted Mean Curvature

Matt Elsey
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Session 1a, Wean 7218
3:20-3:40

Regularity of Solutions to the Liquid Crystals Systems in $\mathbb{R}^2$ and $\mathbb{R}^3$

Mimi Dai
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Session 1b, WeH 8220
3:20-3:40

Advances in Multiscale Kinetic Modeling of Grain Growth in Polycrystals

Maria Emelianenko
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Session 1a, WeH 7218
3:40-4:00

Phase and Bifurcation Analysis of a Mean-Field Model for Biaxial Nematic Liquid Crystals

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CONTRIBUTED TALKS
Thursday, May 26

Session 1b, Wean 8220
3:40-4:00

An Entropy Based Theory of the Grain Boundary Character Distribution

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Coffee Break
4:00-4:20, Wean 6220

Session 2a, Wean 7218
4:20-4:40

Multiscale Atomistic Modeling of Ferroelectrics

Jason Marshall
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Session 2b, Wean 8220
4:20-4:40

Analytical and Numerical Results for Brownian Motion Through a Material

Carey Caginalp
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Session 2a, Wean 7218
4:40-5:00

Variational Theory for the Peridynamics Model

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CONTRIBUTED TALKS
Thursday, May 26

Session 2b, Wean 8220
4:40-5:00

Temper Coarse-Graining of ODE Systems using Parametrized Locally Invariant Manifolds

Likun Tan
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Session 2a, Wean 7218
5:00-5:20

Multiscale Modeling in Peridynamic Solid Mechanics

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Session 2b, Wean 8220
5:00-5:20

Heat Conduction of Fractional Cattaneo Type

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Session 2a, Wean 7218
5:20-5:40

Mathematical Analysis of the Nonlocal State Based Peridynamic Models

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CONTRIBUTED TALKS
Friday, May 27

Session 3a, Wean 7218
3:00-3:20

Singular Perturbation Models in Phase Transitions for Second Order Materials

Milena Chermisi
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Session 3b, Wean 8220
3:00-3:20

The further From the Defect the Stronger Electric and Mechanical Fields – Analysis of a Green's Function in Piezoelectrics

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Session 3a, Wean 7218
3:20-3:40

A Discrete Phase Field Model with Microscopic Potential

Emre Esenturk
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Session 3b, Wean 8220
3:20-3:40

Links Between Effective Tensors of Fiber-Reinforced Elastic Composites

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CONTRIBUTED TALKS
Friday, May 27

Session 3a, Wean 7218
3:40-4:00

Phase Field Modeling for Heterogeneous Materials by Differential Variational Inequality

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Session 3b, Wean 8220
3:40-4:00

Periodic Homogenization for a Model of Plasticity

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Coffee Break
4:00-4:20, Wean 6220

Session 4a, Wean 7218
4:20-4:40

From Particles to Non-equilibrium Thermodynamics: A New Perspective

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Session 4b, Wean 8220
4:20-4:40

Mathematical Challenges in Magma Dynamics

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CONTRIBUTED TALKS
Friday, May 27

Session 4a, Wean 7218
4:40-5:00

Variational Characterization of the Effective Yield Set in Polycrystal Plasticity

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Session 4b, Wean 8220
4:40-5:00

Boundary Layer for Viscoelastic Fluids

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Session 4a, Wean 7218
5:00-5:20

Simulations of Vanishing Capillarity Limits for Kohn-Müller and Aviles-Giga Type Models

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Session 4b, Wean 8220
5:00-5:20

Shrinking Dimer Dynamics and its Applications

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Session 4a, Wean 7218
5:20-5:40

Microstructure in Solids as a Curve of Maximal Slope

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CONTRIBUTED TALKS
Friday, May 27

Session 4b, Wean 8220
5:20-5:40

Objective Molecular Dynamics Study of Mechanical Properties of Carbon Nanotubes

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