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IMA NEWSLETTER # 337

1–30 November 2004

2004–2005 Program

MATHEMATICS OF MATERIALS AND MACROMOLECULES: MULTIPLE SCALES, DISORDER, AND SINGULARITIES

See www.ima.umn.edu/matter for a full description of the 2004–2005 program on Mathematics of Materials and Macromolecules: Multiple Scales, Disorder, and Singularities

IMA schedules are subject to revision, particularly during workshops. See www.ima.umn.edu/~seminar/sched and www.ima.umn.edu/newsletters for the latest scheduling information.

PART I: News and Notes

<p>IMA Symposium:</p>

<p>Prospects for Mathematics and Mechanics upon the 80th Birthday of Jerry Ericksen</p>
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<p>November 5–6, 2004</p>

<p>Organizers: Millard F. Beatty (University of Nebraska – Lincoln), Yi-chao Chen (University of Houston), Richard D. James (University of Minnesota), Mitchell Luskin (University of Minnesota)</p>
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<p>See www.ima.umn.edu/matter/fall/ericksen.html</p>

Jerry Ericksen pioneered the development of continuum theory for complex materials and laid the groundwork for theory that bridges continuum mechanics and molecular structure. Ericksen's work makes use of, and has led to the development of, new lines of thought in mathematics, especially in PDEs and geometry. He has inspired both scientists and mathematicians, his influence reaching deeply into both pure mathematics and materials science. This forward-looking symposium celebrates his accomplishments, and seeks to identify prospects for future research on nonlinear materials.

PARTICIPATING INSTITUTIONS: Consiglio Nazionale delle Ricerche, Georgia Institute of Technology, Indiana University, Iowa State University, Kent State University, Lawrence Livermore National Laboratory, Los Alamos National Laboratory (LANL), Michigan State University, Mississippi State University, Northern Illinois University, Ohio State University, Pennsylvania State University, Purdue University, Rice University, Sandia National Laboratories, Seoul National University (BK21 Math-SNU), Statistical Research Center for Complex Systems (SRCCS) at Seoul National University, Texas A&M University, University of Chicago, University of Cincinnati, University of Delaware, University of Houston, University of Illinois (Urbana), University of Iowa, University of Kentucky, University of Maryland, University of Michigan, University of Minnesota, University of Notre Dame, University of Pittsburgh, University of Texas at Austin, University of Wisconsin, University of Wyoming, Wayne State University.

PARTICIPATING CORPORATIONS: Boeing, Corning, ExxonMobil, Ford, GE, General Motors, Honeywell, IBM, Johnson & Johnson, Lockheed Martin, Lucent, Motorola, Schlumberger, Siemens, Telcordia Technologies, 3M.

Version of November 1, 2004

IMA Workshop:
Future Challenges in Multiscale Modeling and Simulation

November 18-20, 2004

Organizers: Thomas Yizhao Hou (California Institute of Technology)
and Mitchell Luskin (University of Minnesota)

See www.ima.umn.edu/matter/fall/challenges.html

Multiscale modeling and simulation has emerged as a new research area which has already had a significant impact on many scientific and engineering disciplines. Despite considerable progress in a wide range of the sciences, and a growing awareness of the importance of multiscale approaches, currently there is fragmentation in multiscale methodology and its rigorous analysis across its areas of application. This workshop will bring leading experts together to discuss the latest developments in their disciplines and describe the future challenges in multiscale modeling and simulation. The workshop will also provide a special opportunity to connect domain experts from scientific and engineering disciplines with specialists in mathematical and computational analysis.

Math Matters: IMA Public Lecture Series:
The Marriage Equation: A Practical Theory for Predicting Divorce and a Scientifically-Based Marital Therapy

November 18 at 7:00 PM in Smith Hall 100

Professor James D. Murray
Emeritus Professor of Mathematical Biology, University of Oxford and Emeritus
Professor of Applied Mathematics, University of Washington

The rise in divorce rates in developed countries, including the US, is a widespread, important and poorly understood phenomenon. Laboratory methods have been developed to observe interactions of couples to identify patterns that are predictive of divorce or whether the couple will be unhappily married. Mathematician James Murray and psychologist John Gottman have developed a marital interaction theory based on key empirical findings from a large number of couples who have been tracked for the past 12 years. Changes over time in the parameters of the model can account for deterioration in a couple's relationship, and how their relationship could cross a threshold after which recovery becomes difficult. With a couple's data they can simulate how this couple may interact under conditions different from those in which they were first observed. The modeling thus leads to "what if" thought experiments which can be used to help design new scientifically-based intervention strategies for troubled marriages.

New Participating Institution: the University of Texas at Austin

The University of Texas at Austin has joined the IMA as a Participating Institution. J. Tinsley Oden, director of the Institute for Computational Engineering and Sciences and Cockrell Family Regents' Chair in Engineering (Aerospace Engineering and Engineering Mechanics), will serve as the IMA Participating Institutions Council representative for the University of Texas.

IMA Website

Comments or suggestions concerning the IMA website may be addressed to webmaster@ima.umn.edu.
In particular, we appreciate any information about World-Wide Web links relevant to current and upcoming IMA programs.

PART II: Schedule for 1–30 NOVEMBER 2004

Monday, November 1

MATERIALS SEMINAR: MULTISCALE FOCUS GROUP, 409 Lind

11:15 **Markos Katsoulakis** Mathematical strategies for stochastic multiscale prob-
University of Massachusetts, Amherst lems: coarse-graining, loss of information and adaptivity

Tuesday, November 2

IMA POSTDOC SEMINAR, 409 Lind Hall

11:15 **Richard McGehee** Some Mathematical Aspects of Cluster Analysis
Mathematics, University of Minnesota

Abstract: Cluster analysis, a data mining technique applied to such diverse areas as marketing, homeland security, and medical research, has a simple mathematical formulation. Although cluster analysis has been in use for at least 35 years, there appear to be some unresolved mathematical questions underlying some of the common computational techniques used for analyzing large data sets. In this lecture, I present an overview of the subject and pose some open questions.

Wednesday, November 3

MATERIALS SEMINAR: SINGULARITIES FOCUS GROUP, 409 Lind Hall

11:15 **Fanghua Lin** Multiple time scale dynamics for a coupled nonlinear
Courant Institute, New York University Schrodinger equations

MATERIALS SEMINAR: SOFT MATTER FOCUS GROUP, 409 Lind Hall

2:30 **David C. Morse** What's wrong with the Langevin equations? Part II
Chemical Engr/Mat Sci, University of
Minnesota

Thursday, November 4

IMAGE PROCESSING AND ANALYSIS WORKING SEMINAR, 409 Lind Hall

12:20 **Dan Kersten** Computational Approaches to Human Object Perception
Psychology, University of Minnesota

Friday, November 5

**IMA SYMPOSIUM: PROSPECTS FOR MATHEMATICS AND MECHANICS UPON THE 80TH BIRTHDAY
OF JERRY ERICKSEN, NOVEMBER 5–6, EE/CS 3-180**

9:50–10:00 **Welcome and Introduction**

10:00–10:45 **Richard D. James** Hysteresis and geometry: a way to search for new materials with “unlikely” physical properties
Aerospace Engr/Mechanics, University of Minnesota

Abstract: These thoughts begin with the observation by physicists, probing new phenomena through the use of first principles’ studies, that the simultaneous occurrence of ferromagnetism and ferroelectricity is unlikely. While these studies do not consider the possibility of a phase transformation, there is a lot of indirect evidence that, if the lattice parameters are allowed to change a little, then one might have co-existence of “incompatible properties” like ferromagnetism and ferroelectricity. Thus, one could try the following: seek a reversible first order phase transformation, necessarily also involving a distortion, from, say, ferroelectric to ferromagnetic phases. If it were highly reversible, there would be the interesting additional possibility of controlling the volume fraction of phases with fields or stress. Thus, one could imagine having a strong magnet; apply stress to it and it becomes a strong ferroelectric. The key point is reversibility.

Even big first order phase changes can be highly reversible (liquid water to ice, some shape memory materials), and we argue that it is the nature of the shape change that is critical. We suggest, based on a close examination of measured hysteresis loops in various martensitic systems, that reversibility is governed by the presence of certain special relations among lattice parameters. While these relations are naively geometric, their fundamental status is not clear, but they likely relate to a concept of metastability for an energy functional that includes both interfacial and bulk energy. Fundamentally, we lack the ability to formulate the appropriate concept of metastability because we do not really understand how to model interfacial energy, as we explain.

Acknowledgment: John Ball, Karin Rabe, Jerry Zhang.

10:45–11:15 **Coffee**

11:15–12:00 **Kaushik Bhattacharya** Ferroelectric ceramics
California Institute of Technology

Abstract: This talk will outline recent progress in understanding ferroelectric perovskite ceramics with an emphasis on their electromechanical behavior.

2:00–2:45 **David Kinderlehrer** Issues for interfaces in polycrystals
Carnegie Mellon University

Abstract: Nearly all technologically useful materials are polycrystalline. Their ability to meet system level specifications of performance and reliability is influenced by the types of grain boundaries present and their connectivity. We explore the role of mesoscale theory and experiment designed to establish predictive models of material behavior. Traditionally we have studied geometry-based statistics, like relative area statistics or distributions of numbers of sides of grains. With the advent of automated data acquisition we now have the possibility of obtaining large quantities of both geometric and crystallographic information. In particular we shall discuss two new results which lead to the astonishing conclusion that a polycrystal may leave its “footprint” in a microscopic scan: simple analysis of the scan reveals the identity of the material.

This is part of the CMU MRSEC project.

2:45–3:15 **Coffee**

3:15–4:00 **Fanghua Lin** TBA
Courant Institute of Mathematical Sciences New York University

4:00–4:30 **Coffee**

4:30 **Round table 1: Jim Casey** A theory of pseudo-rigid bodies
University of California – Berkeley

Abstract: Bodies that are somehow capable of keeping their deformation fields homogeneous have been studied extensively in the literature. Such “pseudo-rigid” bodies, or “Cosserat points”, have been used successfully in a variety of applications. The main question addressed in this lecture is: How, in principle, can a 3-dimensional continuum, subjected to arbitrary applied loads, keep its deformation field homogeneous? The homogeneity condition is regarded as a “global constraint”, and a system of indeterminate reactive stresses is introduced. The remaining part of the stress tensor is specified by a constitutive equation. The reactive stresses play the same role as in rigid body dynamics. It is also shown how a pseudo-rigid body can be represented by a point moving in a 12-dimensional Euclidean space, the metric of which is determined by the radius of gyration of the body. In the presence of holonomic constraints, the configuration manifold is Riemannian, and a set of Lagrange’s equations emerge as the covariant components of the governing balance equation.

5:00 **Round table 2: Howard Brenner** Navier-Stokes-Fourier revisited
Massachusetts Institute of Technology

Abstract: This talk builds upon the pioneering work of Dan Joseph and co-workers in clarifying the notion of what is meant by an “incompressible” fluid when density gradients are present. In particular, we introduce the notion of volume as an extensive transportable physical property of a fluid continuum in both liquids and gases. Of special interest is the kinematical notion of the “diffuse” transport of volume, above and beyond the conventional (albeit implicit) view of convective volume transport, the latter being simply and inseparably linked to mass transport through the agency of the fluid’s density; that is, in the presence of density gradients, volume can be transported through space without a concomitant movement of mass. Beyond the purely kinematical aspects of volume transport reflected in the work of Joseph et al., the diffuse transport of volume is accompanied by both momentum and energy transport in amounts above and beyond the amounts heretofore considered in standard continuum-mechanical theories of diffuse momentum and energy transport. This leads to constitutive revisions of both Newton’s law of viscosity governing the diffuse transport of momentum and Fourier’s law of heat conduction governing the diffuse transport of energy (the latter when a clear distinction is drawn between the respective fluxes of heat and internal energy). Experimental evidence based upon the phenomena of thermophoresis and thermal transpiration in single-component gases undergoing heat transfer, together with replacement of the no-slip mass-velocity condition by a comparable no-slip volume-velocity condition, is used to quantitatively support the proposed constitutive revisions to Newton’s and Fourier’s laws.

Saturday, November 6

**IMA SYMPOSIUM: PROSPECTS FOR MATHEMATICS AND MECHANICS UPON THE 80TH BIRTHDAY
OF JERRY ERICKSEN, NOVEMBER 5–6, EE/CS 3-180**

10:00–10:45 **Lev Truskinovsky** Thermodynamics of rate independent plasticity
Ecole Polytechnique, Palaiseau

Abstract: We show that the singular dissipative potential of the phenomenological rate independent plasticity can be obtained by homogenization of a micro-model with quadratic dissipation. The essential ingredient making this reduction possible is a rugged energy landscape at the micro-scale, generating under external loading a regular cascade of subcritical bifurcations. Such landscape may appear as a result of a sufficiently strong pinning or jamming of defects, leading to elastic micro-metastability. The rate independent plastic deformation emerges in this description as a continuous succession of infinitesimal viscous events; the limiting procedure presumes the elimination of small time and length scales. We present an explicit example of a simple viscoelastic mass-spring system whose macroscopic dissipative behavior is plastic rate independent.

10:45–11:15 **Coffee**

11:15–12:00 **Masao Doi** A variational principle in dissipative systems
University of Tokyo

Abstract: In constructing kinetic equations which describe the motion of complex fluids (fluid mixtures, liquid crystals, polymer solutions and gels), thermodynamics gives us an important guide. The way how one uses the principle of thermodynamics, however, seems to have various versions. In this talk, I would like to discuss a way which I found useful. It is based on Rayleigh's extension of the Lagrangian mechanics to dissipative systems. In this talk, I explain the method and discuss its applications to several systems (two fluid model, electrolyte solutions, gels etc).

2:00–2:45 **Patricia E. Cladis** TBA
Advanced Liquid Crystal Technologies

2:45–3:30 **Coffee**

3:30 **Round table 3: Anna Vainchtein** Kinetics of lattice phase transitions
University of Pittsburgh

Abstract: Understanding the origin of energy dissipation and the associated kinetics of phase boundaries remains an important open problem in modeling lattice phase transitions in martensites. Following the pioneering work of Ericksen [1975], it has become common to model these materials by an up-down-up stress-strain relation in the framework of continuum elasticity theory. The corresponding dynamic problem changes type and is ill-posed; however, it may be regularized by prescribing an additional kinetic relation between the driving force and the velocity of a phase boundary. This relation is usually either postulated or derived from a phenomenological model accounting for dispersive and dissipative effects.

In this talk we will describe how one can avoid introducing additional phenomenological parameters and instead obtain a kinetic relation by replacing the continuum model with its natural discrete analog. We consider a lattice model of martensitic phase transition which takes into account long-range interactions of an arbitrary range. Although the model is Hamiltonian at the microscale, it generates a nontrivial macroscopic kinetic relation. The apparent dissipation is due to the induced radiation of lattice waves carrying energy away from the front.

This is joint work with Lev Truskinovsky (Ecole Polytechnique, France).

4:00 **Round table 4: Gianni Royer-Carfagni** The role of stress on chemical transformations in an elastic bar with nonconvex chemomechanical free energy
Universita di Parma (CNR)

Abstract: The equilibrium of an elastic bar capable of undergoing chemomechanical transformations and in contact with a chemically aggressive environment is considered. In the proposed model, stable equilibrium states are identified with minimizers of a specific free energy functional, which depends upon the axial strain of the bar and the extent of reaction with an external agent, which is dispersed in a surrounding vapor or liquid solution with assigned chemical potential. In general, the corresponding minimization problem is nonconvex and, therefore, it predicts the coexistence of equilibrium phases. This work is related to the now classical problem of Ericksen for an elastic bar stretched in either a "hard" or a "soft" testing machine. However, here, the presence of an additional internal variable, which represents the extent of reaction, allows for phase transformations which are stress-induced and/or driven by changes in the chemical composition of the surrounding environment. We discuss a characterization of "hard" or "soft" environmental chemical boundary conditions. The model is germane to the description of several phenomena, such as the swelling of ionic gels under chemomechanical actions, or the formation of expanding crusts in stone monuments due to acid rain or an otherwise polluted atmosphere.

4:30 **Round table 5: Anja Schlömerkemper** About magnetic force formulae
Universität Stuttgart

Abstract: The formula for the magnetic force that is exerted by a magnetic field on a single magnetic dipole is well accepted. On the other hand, the formulation of magnetic force formulae for macroscopic magnetic systems has been under debate for a long time. A final answer to this question is of interest in the context of deformable magnetic bodies as, for instance, of ferromagnetic shape memory alloys.

In the first part of the talk, a brief overview of Brown's [1] approach is given and related work that was initiated by Brown's

approach is mentioned.

Secondly, we focus on the formula for the magnetic force between rigid magnetic bodies which was derived from a lattice of magnetic dipoles in a continuum limit [2]. The main ideas of this approach and of the mathematical proof are presented. In addition to the classical magnetic force formulae, one obtains a surface force density which depends on the underlying lattice structure and includes short range contributions of the magnetic interaction at interfaces.

In the final part of the talk we address the question of whether this magnetic force formula describes nature well and compare it with Brown's formula.

[1] Brown, W.F., Magnetoelastic Interactions, Springer-Verlag, Berlin, 1966

[2] Schlmerkemper, A., Mathematical derivation of the continuum limit of the magnetic force between two parts of a rigid crystalline material, accepted for publ. in Arch. Rational Mech. Anal.

5:00	Weisman Art Museum open for viewing	Banquet attendees only
6:00	Reception at Weisman Art Museum	Banquet attendees only
6:30	Seating for Dinner at Weisman Art Museum	

Monday, November 8

MATERIALS SEMINAR: MULTISCALE FOCUS GROUP, 217 Lind Hall

11:15	James Sethna Cornell University	TBA
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Tuesday, November 9

IMA POSTDOC SEMINAR, location TBA

11:15	Peter Sternberg Indiana University	Elliptic Variational Problems on Constricted Networks with Applications to Ginzburg-Landau Theory
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Abstract: I will analyze variational problems set on a network of thin constricted tubes. In the asymptotic regime where the tubes collapse to a graph, one can identify a one dimensional variational problem with interesting natural boundary conditions at the nodes which in particular encourage jumps in the (limit of) minimizers across the various branches of the graph. An application to tunneling across weak links in a superconductor will be discussed.

Thursday, November 11

IMAGE PROCESSING AND ANALYSIS WORKING SEMINAR, 409 Lind Hall

12:20	Xiaoru Yuan Computer Science, U of M	Procedural Image Processing for Non-photorealistic Rendering and Visualization
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Friday, November 12

MATERIALS SEMINAR: SOFT MATTER FOCUS GROUP, 409 Lind Hall

11:15 **Georg Dolzmann** TBA
University of Maryland College Park

IMA/MCIM INDUSTRIAL PROBLEMS SEMINAR, 570 Vincent Hall

1:25 **James Greenleaf** Quantitative Promise of Vibro-acoustography and Vibrometry
Mayo Clinic, Rochester, MN

Abstract: Vibro-acoustography is a method of imaging and measurement that uses ultrasound radiation force to vibrate objects. The radiation force is concentrated laterally by focusing the ultrasound beam. The radiation force is limited in depth by intersecting two beams at different frequencies so that there is interference between the beams at the difference frequency only at their intersection. This results in a cyclic radiation stress of limited spatial extent on or within the object of interest. The resulting harmonic displacement of the object is detected by its acoustic emission, with ultrasound Doppler measurement, with a laser interferometer or the resulting acoustic emission is detected with a hydrophone. The displacement is a complicated function of the object material parameters. However, significant low speckle and high contrast images and measurements can be made with this arrangement. Vibro-acoustography can produce images of biologically relevant objects such as breast microcalcification, vessel calcifications, heart valves, and normal arteries. In addition vibrations placed in specific geometrically shaped tissues such as arteries can be used to induce modal responses that can be used to solve for material properties. Specific examples of these results will be described.

Monday, November 15

MATERIALS SEMINAR: MULTISCALE FOCUS GROUP, 409 Lind Hall

11:15 **Xiantao Li** A multiscale model for the dynamics of solids at finite temperature
IMA Postdoc

Abstract: I will present a multiscale method for the modeling of dynamics of solids at finite temperature. In this method, the molecular dynamics is reformulated to the form of conservation laws, which are to be coupled with macroscale descriptions. I will specifically discuss the following issues:

1. extracting constitutive or kinetic relations from atomistic models,
2. nonreflective boundary conditions,
3. interface between atomistic/continuum,
4. error estimate as a guideline for mesh adaption,
5. application to phase transformation and dynamic fracture mechanics.

Thursday, November 18

**IMA WORKSHOP: FUTURE CHALLENGES IN MULTISCALE MODELING AND SIMULATION,
NOVEMBER 18–20, EE/CS 3-180**

8:30 **Registration and Coffee**

9:05-9:20 **D.N. Arnold and organizers** Opening Remarks

9:20-9:50 **Richard D. James** TBA
University of Minnesota

10:00-10:30 **Felix Otto** TBA
Universität Bonn

10:40-11:10 **Coffee**

11:10-11:40 **Emily A. Carter** Challenges for Quantum-Mechanics-Based Multiscale
Princeton University Modeling

Abstract: In principle, the predictive power of multiscale modeling will be greatly enhanced if information is provided by first principles methods that do not rely on input from experiment. However, such methods, especially for metallic systems, are extremely expensive to use. We have recently shown (Fago et al., Phys. Rev. B, 2004) that it is possible to couple a linear scaling density functional theory (DFT) method to the local quasicontinuum method, thereby providing an on-the-fly two-scale method with feedback to both scales. The current state of development of this orbital-free density functional theory (OFDFT) method will be described, including achievements and limitations. We will give an honest appraisal of what the challenges are and how we hope to overcome them, such that predictive, on-the-fly multiscale modeling will eventually be possible.

12:00 **Lunch**

2:00–2:30 **Andrew Stuart** Conditional Path Sampling of SDEs and the Langevin
University of Warwick MCMC Method

Abstract: We describe a stochastic PDE based approach to sampling paths of SDEs, conditional on observations. The SPDEs are derived by generalizing the Langevin MCMC method to infinite dimensions. Various applications are described including sampling paths subject to two end point conditions (bridges) and nonlinear filter/smoothers.

2:40–3:10 **Folkmar Bornemann** Energy Level Crossings in Molecular Dynamics—Is there
Munich University of Technology a (Mathematical) Passage?

Abstract: We discuss the mathematical description of the quantum dynamics of a molecular system that undergoes a conical intersection of energy levels. At such intersections, because of nonlinear scale-interactions, leading order transitions occur that are the reason for many important reaction mechanisms studied in quantum chemistry. We will review recent work that could help to develop mathematical well-founded versions (without any ad-hoc devices) of the surface-hopping algorithms for the simulation of such systems. We will focus on several challenging open problems.

3:20-3:50 **Coffee**

3:50-4:20 **Yannis G. Kevrekidis** Some Computational Examples of Equation-Free Model-
Princeton University ing

Abstract: I will discuss a number of modeling examples whose computation is facilitated in an equation-free multiscale framework. The examples range from MC computations of micelle formation to agent based simulation and studies of coupled oscillators. I will also present some examples of equation-free dynamic renormalization computations.

4:30-5:00 **Open Discussion**
moderated by Robert Kohn

IMAGE PROCESSING AND ANALYSIS WORKING SEMINAR, 409 Lind Hall

12:20 **Bin He** Electrophysiological Neuroimaging
Biomedical Engineering, U of M

Friday, November 19

**IMA WORKSHOP: FUTURE CHALLENGES IN MULTISCALE MODELING AND SIMULATION,
NOVEMBER 18–20, EE/CS 3-180**

9:00 **Coffee**

9:20-9:50 **Bjorn Engquist** TBA
Princeton University

10:00-10:30 **Thomas Yizhao Hou** Multiscale Modeling and Computation of Incompressible
California Institute of Technology Flow

Abstract: We perform a systematic multiscale analysis for incompressible Euler equations with rapidly oscillating initial data. The initial condition for velocity field is assumed to have a two-scale structure. One of the important questions is how the two-scale velocity structure propagates in time and whether nonlinear interaction will generate more scales dynamically. By making an appropriate multiscale expansion for the velocity field, we show that the two-scale structure is preserved dynamically. Further, we derive a well-posed homogenized equation for the 2-D and 3-D incompressible Euler equations. Our multiscale analysis also reveals an interesting structure of the Reynolds stress, which provides useful guideline in designing systematic coarse grid model for the incompressible flow.

10:40-11:10 **Coffee**

11:10–11:40 **Olivier Pironneau** Nuclear Waste Safety of Repository Vaults: A Multi-Scale
Université Paris VI Problem

Abstract: This analysis explores the possibilities of multiscale expansions and domain decomposition to solve part of the Couplex 1 exercise posed by the French agency for nuclear waste, ANDRA. We concentrate on the hydrostatic pressure and show that the slenderness of the domain and the large variations of the Darcy constants allows an analytical approximation which our test reveals to be true to relative errors smaller than 1/1000. The numerical tests are done in 2D with freefem+ and in 3D with freefem3D, both in the public domain. Some considerations will be also given for Iodine transport.

12:00 **Lunch**

2:00–2:30 **Russel Caflisch** Multiscale Modeling of Epitaxial Growth Processes
UCLA

Abstract: Epitaxy is the growth of a thin film by attachment to an existing substrate in which the crystalline properties of the film are determined by those of the substrate. No single model is able to address the wide range of length and time scales involved in epitaxial growth, so that a wide range of different models and simulation methods have been developed. This talk will review several of these models - kinetic Monte Carlo (KMC), island dynamics and continuum equations - in the context of layered semiconductors applied to nanoscale devices. We describe a level set method for simulation of the island dynamics model, validation of the model by comparison to KMC results, and the inclusion of nucleation and strain. This model uses both atomistic and continuum scaling, since it includes island boundaries that are of atomistic height, but describes these boundaries as smooth curves.

2:40-3:10 **Weinan E** Simple Concepts in Multiscale Modeling
Princeton University

Abstract: What is multiscale modeling about and why is there such a huge interest right now? These questions are less trivial than one might initially think, given that almost every problem in nature is multiscaled, and there has already been a long history of using multiscale ideas in scientific computing. We will discuss these questions in the context of several canonical multiscale problems and multiscale methods. This allows us to give a candid assessment of the current status of multiscale modeling in several areas.

3:20–3:50 **Coffee**

3:50–4:20

Achi Brandt
UCLA

From Fast Solvers to Systematic Upscaling

Abstract: Most numerical methods for solving large-scale systems tend to be extremely costly, for several general reasons, each of which can in principle be removed by multiscale algorithms. Algorithms to be briefly surveyed: fast multigrid solvers for discretized partial-differential equations (PDEs) and for most other systems of local equations; fast summation of long-range (e.g., electrostatic) interactions and fast solvers of integral and inverse PDE problems; collective computation of many eigenfunctions; slowdown-free Monte Carlo simulations; multilevel methods of global optimization; and general procedures for “systematic upscaling”.

SYSTEMATIC UPSCALING is a methodical approach for deriving, scale after scale, collective variables and governing numerical equations (or transition probabilities rules) at increasingly larger scales, starting from a microscopic scale where first-principle laws are known. Iterating back and forth between all levels allows the computation at each scale to be short and confined to small “windows.”

The multiscale methods are key to removing computational bottlenecks in many areas of science and engineering, such as: QCD (elementary particle) computation; ab-initio quantum chemistry real-time path integrals; density-functional calculation of electronic structures; molecular dynamics of fluids, materials and macromolecules; turbulent flows; tomography (medical-imaging reconstruction); image segmentation and picture recognition; and various large-scale graph optimization, clustering and classification problems. Future directions will be outlined.

4:30–5:00

Open Discussion
moderated by Mitchell Luskin

Saturday, November 20

**IMA WORKSHOP: FUTURE CHALLENGES IN MULTISCALE MODELING AND SIMULATION,
NOVEMBER 18–20, EE/CS 3-180**

9:00

Coffee

9:20-9:50

James P. Sethna
Cornell University

TBA

10:00-10:30

Ken A. Dill
University of California - San Francisco

Protein Folding as a Global Optimization Problem

Abstract: A protein is a chain molecule having a large number of degrees of freedom. In its biological state, it is folded into a single conformation, out of a large conformational space. Finding its native state is a global optimization problem that the protein can often solve in nanoseconds. We have studied how the protein finds its global optimum so quickly, and are exploiting the same strategies for use in computational protein structure prediction.

10:40-11:10

Coffee

11:10-11:40

Linda R. Petzold
University of California – Santa Barbara

Multiscale Stochastic Simulation Algorithm with Stochastic Partial Equilibrium Assumption for Chemically Reacting Systems

Abstract: In microscopic systems formed by living cells, small numbers of reactant molecules can result in dynamical behavior that is discrete and stochastic rather than continuous and deterministic. In simulating and analyzing such behavior it is essential to employ methods that directly take into account the underlying discrete stochastic nature of the molecular events. This leads to an accurate description of the system that in many important cases is impossible to obtain through deterministic continuous modeling (e.g. ODE’s). Gillespie’s Stochastic Simulation Algorithm (SSA) has been widely used to treat these problems. However as a procedure that simulates every reaction event, it is prohibitively inefficient for most realistic problems. We report on our progress in developing a multiscale computational framework for the numerical

simulation of chemically reacting systems, where each reaction will be treated at the appropriate scale. We introduce a stochastic partial equilibrium approximation which is valid even if the population of a fast chemical species is very small, and present some preliminary numerical results from a multiscale numerical simulation.

12:00	Lunch	
2:00–2:30	Zhiming Chen Academy of Sciences	On the Upscaling of a Class of Nonlinear Parabolic Equations
2:40–3:10	Grégoire Allaire Centre de Mathématiques Appliquées, Ecole Polytechnique	Examples of Multiscale Methods in Shape Optimization

Abstract: We discuss two examples of multiscale methods in the context of structural optimization. The first method, which is by now classical, is the homogenization method based on the use of composite materials. Instead of optimizing the position of macroscopic boundaries, the homogenization method optimizes the layout of microscopic holes in a porous material. The two design parameters are the local volume fraction of material and the local microstructure or shape of the holes. The latter one is optimized at a mesh subscale level. The second method is the more recent level set method which relies on the classical Hadamard method of shape sensitivity. Although the level set method is able to handle topology changes, it can not easily nucleate new holes. Therefore it has been coupled with the topological asymptotic method which decides when and where it is favorable to cut an infinitesimal new hole. In these two examples a macroscopic shape optimization process is coupled with a microscopic evaluation, either of the optimal hole microgeometry, or of the potential gain in hole nucleation. In both cases their multiscale characters improve the ability of the algorithms to escape from local minima. Numerical examples in 2-d and 3-d will support this claim.

3:20-3:50	Coffee	
3:50-4:50	Panel Discussion moderated by Yanis Yortsos	
4:50-5:00	Concluding Remarks	

IMA/MCIM INDUSTRIAL PROBLEMS SEMINAR, 570 Vincent Hall

1:25	Maria Ponomorenko University of Minnesota	TBA
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Monday, November 22

MATERIALS SEMINAR: MULTISCALE FOCUS GROUP, 409 Lind

11:15	Petr Plechac Warwick University	TBA
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Monday, November 29

MATERIALS SEMINAR: MULTISCALE FOCUS GROUP, 409 Lind

11:15

Richard D. James TBA
Aerospace Engr/Mechanics, University
of Minnesota

PART III: Current IMA Participants

FIRST YEAR POSTDOCTORAL MEMBERS

Brian DiDonna, Sookyung Joo, Richard Kollar, Matthias Kurzke, Frederic Legoll, Xiantao Li.

SECOND YEAR POSTDOCTORAL MEMBERS

Gerard Awanou, Tim Garoni, Lea Popovic.

POSTDOCTORAL MEMBERS IN INDUSTRIAL MATHEMATICS

Qianying Chen (ExxonMobil), Chuan-Hsiang Han (Ford), Chiu Yen Kao (VA Medical Center), Peter Philip (Corning).

LONG TERM VISITORS

Maria Carme Calderer	University of Minnesota	9/1/2004–6/30/2005
Zhiming Chen	Chinese Academy of Sciences	11/10/2004–11/30/2004
L. Pamela Cook	University of Delaware	9/7/2004–12/31/2004
Masao Doi	University of Tokyo	9/18/2004–12/1/2004
Georg Dolzmann	University of Maryland	10/31/2004–11/21/2004
Matthias Gobbert	University of Maryland – Baltimore County	8/25/2004–12/24/2004
Robert Gulliver	University of Minnesota	9/1/2004–6/30/2005
Weimin Han	University of Iowa	9/1/2004–6/30/2005
Richard D. James	University of Minnesota	9/1/2004–6/30/2005
Markos A. Katsoulakis	University of Massachusetts	10/23/2004–11/22/2004
Martin Kruzik	Czechoslovakian Academy of Sciences	11/7/2004–11/21/2004
Fanghua Lin	New York University	9/1/2004–12/31/2004
Chun Liu	Pennsylvania State University	9/1/2004–6/30/2005
Zuhan Liu	Xuzhou Normal University	9/14/2004–1/31/2005
John Lowengrub	University of California – Irvine	10/20/2004–11/20/2004
Mitchell Luskin	University of Minnesota	9/1/2004–6/30/2005
Jonathan C. Mattingly	Duke University	11/18/2004–12/14/2004
Christof Melcher	Humboldt/Universität zu Berlin	10/17/2004–11/7/2004
Govind Menon	University of Wisconsin	9/7/2004–12/15/2004
Petr Plechac	University of Warwick	9/1/2004–12/31/2004
Rolf Ryham	Pennsylvania State University	9/1/2004–6/30/2005
George R. Sell	University of Minnesota	9/1/2004–6/30/2005
James Sethna	Cornell University	11/5/2004–11/21/2004
Tien-Tsan Shieh	Indiana University	9/1/2004–6/30/2005
Peter J. Sternberg	Indiana University	8/15/2004–6/30/2005
Vladimir Sverak	University of Minnesota	9/1/2004–6/30/2005
Peter Takac	Universität Rostock	10/15/2004–12/15/2004
Zhi Qiang Wang	Utah State University	9/1/2004–12/31/2004
Stephen J. Watson	Northwestern University	9/1/2004–6/30/2005
Olaf Weckner	Massachusetts Institute of Technology	11/16/2004–12/14/2004
Baisheng Yan	Michigan State University	9/1/2004–6/30/2005
Emmanuel Yomba	University of Ngaoundéré	10/6/2004–3/30/2005
Giovanni Zanzotto	University of Padua	11/4/2004–11/21/2004

VISITORS IN RESIDENCE (as of November 1, 04)

Rohan Abeyaratne	Massachusetts Institute of Technology	11/4-6
Gregoire Allaire	Ecole Polytechnique	11/17-21
Kumud S. Altmayer	University of Arizona	11/17-20
Enrico Babilio	University of Pittsburgh	11/4-6
Romesh Batra	Virginia Polytechnic Institute and State University	11/4-6
Patricia Bauman	Purdue University	11/10-23
Millard Beatty	University of Nebraska – Lincoln	11/4-6
Daniel E. Bentil	University of Vermont	11/17-21
Kaushik Bhattacharya	California Institute of Technology	11/4-7
Folkmar Bornemann	Munich University of Technology	11/17-20
Achi Brandt	Weizmann Institute of Science	11/16-21
Howard Brenner	Massachusetts Institute of Technology	11/4-6
Russel Cafilisch	University of California – Los Angeles	11/18-19
Enrico Capobianco	Boston University	11/18-21
Donald Carlson	University of Illinois – Urbana/Champaign	11/4-7
Emily Carter	University of California – Los Angeles	11/17-20
Jim Casey	University of California – Berkeley	11/4-6
Paolo Cermelli	CNR/Universita di Torino	10/24-11/3
Yi-Chao Chen	University of Houston	11/4-7
Ravi Chinnappan	Ford Motor Company	11/17-21
Shue-Sum Chow	Brigham Young University	11-17-20
Patricia Cladis	Advanced Liquid Crystal Technologies	11/4-6
Eric Darve	Stanford University	11/17-21
Cesare Davini	University of Udine	11/4-6
Raffaella De Vita	University of Pittsburgh	11/4-7
Diane L. Denny	University of Wyoming	11/17-20
Luca Deseri	University of Ferrara	11/4-6
Ken A. Dill	University of California – San Francisco	11/17-20
Weinan E	Princeton University	11/17-21
Yalchin Efendiev	Texas A & M University	11/17-21
Marek Elzanowski	Portland State University	11/4-6
Bjorn Engquist	Princeton University	11/17-20
Jerald Ericksen		11/3-7
M. Gregory Forest	University of North Carolina	11/15-20
Roger Fosdick	University of Minnesota	11/5-6
Gilles Andre Francfort	Universite Paris 13	11/17-20
Avner Friedman	Ohio State University	11/13-16
Armenak Socratovich Gasparyan	Program Systems Institute of RAS	11/17-20
James F. Greenleaf	Mayo Clinic /Foundation	11/11-12
Rohit Gupta	University of Minnesota	11/18-20
Robert Hardt	Rice University	11/4-6
Takumi Hawa	University of Maryland	11/17-21
Michael A. Heroux	Sandia National Laboratories	11/17-20
Denis Hirschfeldt	Indiana University	11/2-8
Thomas Yizhao Hou	California Institute of Technology	11/17-20
Yinlun Huang	Wayne State University	11/18-21
Michel E. Jabbour	University of Kentucky	10/25-11/3
Daniel Joseph	University of Minnesota	11/4-6
Ning Ju	Oklahoma State University	11/18-21
Markos A. Katsoulakis	University of Massachusetts	11/17-20
Yannis G. Kevrekidis	Princeton University	11/17-20
David Kinderlehrer	Carnegie Mellon University	11/4-6
Robert V. Kohn	New York University – Courant Institute	11/17-20
Yuen Yick Kwan	Purdue University	11/17-21

Luigi La Ragione	Cornell University	11/17–21
Christopher J. Larsen	Worcester Polytechnic Institute	11/17–21
Richard Lehoucq	Sandia National Laboratories	11/16–20
Bo Li	University of California – San Diego	11/4–6
Xiaofan Li	Illinois Institute of Technology	11/17–20
Yi Li	University of Iowa	11/4–06
Robert P. Lipton	Louisiana State University	11/17–20
Irene Livshits	Ball State University	11/17–21
Helen H. Lou	Lamar University	11/18–20
Gearoid P. Mac Sithigh	University of Missouri – Rolla	11/4–6
Chi-Sing Man	University of Kentucky	11/4–6
Dionisios Margetis	Massachusetts Institute of Technology	11/17–21
Richard P. McGehee	University of Minnesota	11/2–2
Willard Miller	University of Minnesota	11/5–6
Peter J. Mucha	Georgia Institute of Technology	11/17–20
James D. Murray	University of Washington	11/17–19
Nilima Nigam	McGill University	11/4–8
Peter J. Olver	University of Minnesota	11/5–6
Daniel Onofrei	Worcester Polytechnic Institute	11/17–20
Marina V. Osipchuk	Guidant Corporation	11/88
Miao-Jung Yvonne Ou	University of Central Florida	11/17–21
David Owen	Carnegie Mellon University	11/4–6
Jinhae Park	University of Minnesota	11/5–6
Jinhae Park	University of Minnesota	11/18–20
Eric Petersen	United Defense LP	11/4–6
Linda R. Petzold	University of California – Santa Barbara	11/17–20
Daniel Phillips	Purdue University	10/24–11/6
Olivier Pironneau	Universit Paris VI	11/17–20
Keith Promislow	Michigan State University	11/17–20
Arun Ram	University of Wisconsin	11/3–4
Gianni Royer-Carfagni	Universita di Parma (CNR)	11/4–6
Jacob Rubenstein	Indiana University	11/3–4
Marcus Sarkis	Worcester Polytechnic Institute	11/17–20
Gilberto Schleinger	University of Delaware	11/16–21
Anja Schlmerkemper	University of Stuttgart	11/4–12
Dongwoo Sheen	Seoul National University (BK21)	11/17–21
Jie Shen	Purdue University	11/9–22
Shagi-Di Shih	University of Wyoming	11/17–21
Valery P. Smyshlyaev	Cambridge University	11/15–20
Scott Spector	Southern Illinois University	11/4–6
Andrew M. Stuart	University of Warwick	11/17–20
De Witt L. Sumners	Florida State University	11/7–8
Yi Sun	Princeton University	11/17–20
Birgit Suttner	Siemens	11/17–20
Bryan Travis	Los Alamos National Laboratory	11/17–20
Lev Truskinovsky	Ecole Polytechnique – Palaiseau	11/4–6
Igor Tsukerman	University of Akron	11/17–20
Anna Vainchtein	University of Pittsburgh	11/3–7
Kodakkal Kannan Viswanathan	Seoul National University (BK21)	11/17–21
David Voss	Western Illinois University	11/17–22
Li-Lian Wang	Purdue University	11/17–20
Hans Weinberger	University of Minnesota	11/5–6
Christian L. Wernz	University of Massachusetts – Amherst	11/16–20
Jon Wilkening	New York University	11/17–20
Steven Matthew Wise	University of California – Irvine	11/17–20
Jon Wolfson	Michigan State University	11/9–10

Christian Wolfsteiner	Chevron Texaco	11/16–20
Christopher Wolverton	Ford Motor Company	11/17–20
Yanis Yortsos	University of Southern California	11/17–19
Peng Yu	Pennsylvania State University	11/17–21
Weigang Zhong	University of Maryland	11/17–20

See also www.ima.umn.edu/people/