

# INSTITUTE FOR MATHEMATICS AND ITS APPLICATIONS

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## IMA NEWSLETTER # 246

January 1-31, 1997

See the Winter, Summer and Fall 1996 IMA Update for a full description of the 1996-97 program on Mathematics in High-Performance Computing.

<b>News and Notes</b>
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<p>IMA Workshop:</p>
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<p><b>Molecular Structure: Dynamics, Geometry and Topology</b></p>
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<p>January 20-23, 1997</p>
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<p>Organizers: Ridgway Scott (Univ. of Houston) and Tamar Schlick (Courant Institute)</p>
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### Improved IMA Home Page

The IMA has substantially improved its home page on the World-Wide Web, accessible through netscape or other web-reading applications at

<http://www.ima.umn.edu>.

The page is continually under construction. We invite comments or suggestions, which may be addressed to

[webmaster@ima.umn.edu](mailto:webmaster@ima.umn.edu).

In particular, we appreciate any information about World-Wide Web links appropriate to current and upcoming IMA programs.

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PARTICIPATING INSTITUTIONS: Centre National de la Recherche Scientifique, Consiglio Nazionale delle Ricerche, Georgia Institute of Technology, Indiana University, Iowa State University, Kent State University, Michigan State University, Northern Illinois University, Ohio State University, Pennsylvania State University, Purdue University, Seoul National University (RIM - GARC), Texas A&M University, University of Chicago, University of Cincinnati, University of Houston, University of Illinois (Chicago), University of Illinois (Urbana), University of Iowa, University of Kentucky, University of Manitoba, University of Maryland, University of Michigan, University of Minnesota, University of Notre Dame, University of Pittsburgh, University of Southern California, University of Wisconsin, Wayne State University.

PARTICIPATING CORPORATIONS: Bellcore, Eastman Kodak, EPRI, Ford, Fujitsu, General Motors, Honeywell, IBM, Lockheed Martin, Motorola, Siemens, 3M.

## Weekly IMA seminar list available by list server

The IMA is happy to offer its e-mail mailing list service. The mailing list “weekly” is a distribution each Thursday of the next week’s schedule of IMA seminars and events. If you wish to subscribe, simply send an e-mail message to `imalists@ima.umn.edu` whose first line is of the form

`subscribe weekly`

If your preferred e-mail address is different from the one from which you are sending the request, the first line should be

`subscribe weekly you@e.mail.address`

The subject line and the rest of the message are ignored. Questions or problems should be sent to `owner-weekly@ima.umn.edu`.

The current weekly schedule is also available on request via `finger seminar@ima.umn.edu`. An updated `.dvi` file of the IMA Newsletter (current and recent) is available by `ftp` or through the world-wide web.

<b>Schedule for January 1–31, 1997</b>
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### Wednesday, January 1

New Year’s Day, a University of Minnesota holiday. IMA offices will be closed.

### Thursday, January 2

### Friday, January 3

### Monday, January 6

### Special Colloquium in room 570 Vincent Hall

2:15 pm	<b>Russel Caffisch</b> UCLA	Theory and Application of Quasi-Monte Carlo Methods
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*Abstract:* Quasi-random sequences are a deterministic alternative to random or pseudo-random sequences. Correlations between the elements of a quasi-random sequence make them more uniform than random numbers, which leads to Monte Carlo integration errors of size  $(\log N)^d N^{-1}$  as opposed to  $N^{-1/2}$  for standard Monte Carlo. This talk will first describe the basic theory of quasi-random sequences, including the bounds on integration error and methods for generating these sequences. Second, we present results from a set of numerical experiments showing the advantages and limitations of quasi-Monte Carlo in integration and simulation problems. Finally, an application to financial analysis, the evaluation of mortgage-backed securities, will be presented. For this problem, quasi-Monte Carlo computations result in substantial speed-up over standard Monte Carlo.

### Tuesday, January 7

### Wednesday, January 8

### Thursday, January 9

### Friday, January 10

### SEMINAR ON INDUSTRIAL PROBLEMS

11:15 am	<b>Walter Willinger</b> AT&T Labs – Research	The Changing Nature of Network Traffic Analysis and Modeling
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*Abstract:* Historically, the areas of traffic data analysis and modeling have suffered from a severe “drought” of data. However, more recently, this drought has been replaced by a “flood” of traffic measurements from today’s high-speed communication networks that keeps increasing in volume and speed. As a result of these changes, network research (in particular, traffic analysis and traffic modeling) has started to adopt concepts that have a long tradition in the physical sciences but have been all but ignored in the social sciences and in the mainstream statistics literature. In this talk, I will illustrate some of these concepts, show how they apply to modern network traffic analysis/modeling, comment on their implications on traffic engineering and performance analysis of current and future high-speed networks, and outline new areas of research in the mathematical and statistical sciences that result from these changes and are of practical importance for network research.

**The seminar meets in the Seminar Room, Vincent Hall 570.**

**Monday, January 13**

**Tuesday, January 14**

**IMA Postdoc Seminar**

2:30 pm	<b>Margaret Cheney</b> Rensselaer Polytechnic Institute	Inverse Problems for a Perturbed Dissipative Half-Space
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*Abstract:* This talk addresses the scattering of acoustic and electromagnetic waves from a perturbed dissipative half-space. First is a discussion of the application that motivated this work and an explanation of how Maxwell’s equations can be reduced to a simpler scalar model. Next is a discussion of three formulations for direct and inverse problems for the half-space geometry. Two of these formulations relate to scattering problems, and the third to a boundary value problem. Next the three inverse problems are shown to be equivalent in a certain sense. Finally, the boundary value problem is used to outline a simple way to formulate a multidimensional layer stripping reconstruction procedure. This procedure, however, must be stabilized before it can become a practical algorithm for solving the inverse problem.

Organizer: Serguei Maliassov

NOTE: The Postdoc Seminar is organized by the IMA postdoctoral members, but all interested IMA participants are very welcome to attend. The Seminar meets in Vincent Hall 570.

**Wednesday, January 15**

**Thursday, January 16**

**Friday, January 17**

**SEMINAR ON INDUSTRIAL PROBLEMS**

11:15 am	<b>Gary X. Li</b> Motorola	Stress-induced warpage and the compensation in a composite micro-accelerometer
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*Abstract:* Mechanical modeling and analysis have been carried out for a fabricated micro-accelerometer. The sensor is designed with composite polysilicon/silicon nitride tether arms to provide a new overall tensile state. The stress distribution in both polysilicon and silicon nitride films, and the resulting structural deformation, have been calculated. Both experimental results and finite element analysis (FEA) of the complete sensor structure show that a consistent upward deflection of the tether structure exists, which causes an offset of the suspended poly plate and results in yield loss and sensor performance degradation. This phenomenon is explained by designing, fabricating, and testing two cantilever beams with cross-sections similar to the actual tether structure. Depending on the beam’s cross-section dimensions, all the cantilever sample also exhibit upward deflection to varying degrees. Theoretical analysis and FEA simulation are conducted for the cantilever beams, and the results compared with experimental data. An analytical formula is provided to optimize the composite polysilicon/silicon-stride tether geometry to minimize or eliminate the undesirable stress induced.

The seminar meets in the Seminar Room, Vincent Hall 570.

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IMA Workshop:  
**Molecular Structure: Dynamics, Geometry and  
Topology**

January 20–23, 1997

Organizers: Ridgway Scott (Univ. of Houston) and  
Tamar Schlick (Courant Institute)

The design or redesign of macromolecules to perform biological or industrial functions requires quantum-mechanical models to be solved. Various approximate models are currently being refined and further developed as the power of available computers increases. Monte Carlo techniques are also becoming feasible for this class of problem. The workshop will combine researchers involved in the development of these diverse techniques and identify mathematical problems for further study.

The structure of macromolecules can often be described as a linear sequence of bonded atoms (*e.g.*, a DNA nucleotide sequence), yet the three-dimensional structure (and resulting function) remain elusive. The “protein folding problem” is one of the simplest to state and yet impossible to solve for molecules of substantial size. Different approaches are being proposed for attacking this problem, ranging from topology, geometry, mechanics, and even artificial intelligence. The workshop will focus on the various mathematical approaches available. Fundamental to the three-dimensional structure is the quantum-mechanically determined local bond structure.

**Monday, January 20**

Martin Luther King’s Birthday, a University of Minnesota holiday. IMA offices may be closed, although staff will be on hand for the workshop.

**Talks today are in the Seminar Room, Vincent Hall 570**

9:00 am	<b>Registration and Coffee</b>	IMA Lounge, Vincent Hall 502
10:00 am	<b>Welcome and Orientation</b>	A. Friedman, R. Gulliver, R. Scott
10:15 am	<b>Tamar Schlick</b> Courant Institute	Molecular Dynamics: An Overview and Recent Work

*Abstract:* Innovative algorithms have been developed during the past decade for simulating Newtonian physics for macromolecules. A major goal is alleviation of the severe requirement that the integration timestep be small enough to resolve the fastest components of the motion and thus guarantee numerical stability. This timestep problem is challenging if strictly faster methods with the same all-atom resolution at small timesteps are sought. Mathematical techniques that have worked well in other multiple-timescale contexts — where the fast motions are rapidly decaying or largely decoupled from others — have not been as successful for biomolecules, where vibrational coupling is strong.

This talk will review general issues that limit the timestep and describe available methods (constrained, reduced-variable, implicit, symplectic, multiple-timestep, and normal-mode-based schemes). Our dual timestep method LN (for its origin in a Langevin/Normal Modes algorithm) will also be presented and recent results presented (joint work with E. Barth and M. Mandziuk). LN relies on an approximate linearization of the equations of motion every  $\Delta t$  interval (5 fs or less), the solution of which is obtained by explicit integration at the inner timestep  $\Delta\tau$  (*e.g.*, 0.5 fs). Since this subintegration process does not require new force evaluations, LN is

computationally competitive, providing 4–5 speedup factors, and results in good agreement, in comparison to 0.5 fs trajectories. In combination with force splitting techniques, even further computational gains can be achieved for large systems.

11:00 am	<b>Coffee Break</b>	IMA Lounge, Vincent Hall 502
11:15 am	<b>Tamar Schlick</b> Courant Institute	Molecular Dynamics: An Overview and Recent Work (cont.)
2:00 pm	<b>Jan Hermans</b> University of North Carolina	Simulations of protein dynamics: Investigations of conformation change and interactions with small molecules

*Abstract:* Simulations of molecular dynamics with classical mechanics and simple empirical force fields give the most accurate representation outside of quantum mechanics, and can today be performed on systems containing many thousands of atoms for periods of simulated time of many nanoseconds. Simulation accuracy has been greatly improved by economical methods for computing long-range electrostatic forces (by our colleagues Board at Duke and Darden at NIEHS). Computer resources have grown so that it is feasible to implement so-called steered molecular dynamics, SMD (implemented at UNC with use of **vmd**, a molecular graphics program from Klaus Schulten’s group at Illinois). In our SMD project we are studying the extraction of a non-covalently bound small molecule from a protein, by a user-specified tug, through any of several likely exit routes, and this is followed by batch calculations of the energetics experienced by a molecule moving naturally along such a path, i.e., by diffusion, rather than as the result of an artificial tug.

Changes in conformation and interactions with small molecules are, of course, intrinsic to the central role played by proteins in biology. We have over the years developed methods to study the energetics of these processes. This work has, for example, shown that the simulations reproduce the experimentally measured equilibria between helix and coil states of polypeptides, and give insight into the interactions that can be held responsible for stabilizing the helix. Rather surprisingly, our results indicate that electrostatic forces contribute nothing to the stability of the helix relative to the coil, but that it is the balance of the van der Waals (packing) forces which favors the helix over the coil. Recently, we have been able to reproduce the binding equilibrium of a small molecule to a protein in terms of its free energy, and to decompose this quantitatively into parts, a binding energy and a “cratic” free energy, the latter corresponding to the loss of positional and orientational freedom when two molecules form a complex.

4:00 pm	<b>IMA Tea (and more!)</b>	Vincent Hall 502 (The IMA Lounge)
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A variety of appetizers and beverages will be served.

## Tuesday, January 21

### Talks today are in Seminar Room Vincent Hall 570

9:00 am	<b>Registration and Coffee</b>	IMA Lounge, Vincent Hall 502
10:00 am	<b>Randy Paffenroth</b> Univ. of Maryland	Software Demonstration

Paffenroth will demonstrate the Autovisualization Application (AVA).

10:30 am	<b>Coffee Break</b>	IMA Lounge, Vincent Hall 502
11:00 am	<b>Robert D. Skeel</b> University of Illinois	Difficulties with Multiple Time Stepping and the Fast Multipole Algorithm in Molecular Dynamics

*Abstract:* Numerical experiments are performed on a 36,000-atom protein–DNA–water simulation to ascertain



*Abstract:* We discuss recent developments in the solution of distance geometry problems that arise in the interpretation of NMR data and in the determination of protein structures. Distance geometry problems give rise to global optimization problems with simple structure, but a large number of local minimizers.

We present algorithms for determining solutions to distance geometry problems, where upper and lower bounds are provided on the distance data. Our approach is based on using the Gaussian transform to map the original objective function into a smoother function with fewer minimizers, and using an optimization algorithm on the transformed function to trace the minimizers back to the original function.

We use limited-memory variable-metric methods and sparse Newton methods to trace solution curves. We present results for distance data derived from DNA protein fragments with up to 2,000 atoms.

This work is joint with Zhijun Wu.

10:30 am	<b>Coffee Break</b>	IMA Lounge, Vincent Hall 502
11:00 am	<b>Zhijun Wu</b> Argonne National Laboratory	Geometrical Structures of Large, Confined Ionic Systems

*Abstract:* We discuss the molecular optimization problem of determining the optimal configurations of large, confined ionic systems. This problem arises in the study of heavy ions in plasma physics, where there is interest in the evolution of the optimal configurations as the size of the system increases. In particular, we are interested in determining the phase transition of the ionic system from the shell structure to the BCC lattice. Based on experimental evidence, scientists expect the phase transition to occur at systems with 200,000 atoms.

We show that for this problem we are able to obtain sharp lower and upper bounds on the value of the potential energy for the optimal configurations. We also study the evolution of the optimal configurations. Our approach is based on using the Gaussian transform to map the original objective function into a smoother function with fewer minimizers, and using an optimization algorithm on the transformed function to trace the minimizers back to the original function.

We discuss the general geometrical properties of optimal ionic systems, and discuss our computational experience with small to medium-sized (2,000 atoms) problems. We present results obtained with the IBM SP and CAVE at Argonne's High-Performance Computing Research Facility.

This work is joint with Jorge Moré.

2:00 pm	<b>Richard A. Friesner</b> Columbia University	A Computational Approach to the Determination of Protein Tertiary Structure Assuming Knowledge of Secondary Structure
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*Abstract:* We have developed a new reduced model potential function for determination of tertiary protein structure assuming knowledge of secondary structure. The model potential uses both alpha-carbon and beta-carbon distance information and is based upon a synthesis of data base statistics, molecular mechanics potentials, and direct optimization of parameters. A key aspect of development of the potential has been minimization of the native structure using an analytical gradient methodology. To perform global optimization, we have implemented a modified version of the branch and bound algorithm proposed by Floudas and coworkers, which appears to be quite powerful for dealing with this type of model. Promising results have been obtained for a significant number of proteins ranging in size from 40 to 180 amino acid residues.

3:00 pm	<b>Coffee Break</b>	IMA Lounge, Vincent Hall 502
	<b>Math Department Seminar on PDEs in room Vincent Hall 211:</b>	
3:35 pm	<b>Shari Moskow</b> MCIM	First order corrections to the homogenized eigenvalues of a periodic composite medium
6:00 pm	<b>Workshop Dinner</b> Radisson Hotel	Alumni Room, second floor

Reception at 6:00 in the Alumni Room, dinner at 6:30.

**Thursday, January 23**

**Talks today are in Seminar Room Vincent Hall 570**

9:00 am	<b>Registration and Coffee</b>	IMA Lounge, Vincent Hall 502
9:30 am	<b>L. Ridgway Scott</b> University of Houston	High-Performance Computation in Biomolecular Modeling

*Abstract:* High-performance computation offers both challenges and opportunities for biomolecular modeling. Numerous standard codes are now available on a wide range of platforms. These codes are being used to do simulations of biologically important systems that are an order of magnitude larger than previously possible, and for a significantly smaller cost. We highlight some of the efforts carried out in our group as part of the National High-Performance Computing and Communication Initiative. Not only is this work having a significant impact on the development of biomolecular science, it is also having a substantial influence on the development of future high-performance computing platforms.

We describe the development of some parallel iterative techniques for solving boundary value problems for elliptic partial differential equations. Using domain decomposition techniques, we have modified standard sequential iterative techniques to obtain effective parallel methods with minimal code restructuring. We contrast implementations on distributed-memory and shared-memory scalable parallel processors. We describe the use of two different programming paradigms, one involving explicit parallelism in a distributed-memory model and the other utilizing simple loop decompositions in a shared-memory model. Our primary conclusion is that parallel computing on existing commercial parallel supercomputers makes it routine to do three-dimensional modeling of biomolecular systems.

We also describe similar successes in parallelizing and using existing codes for molecular dynamics. One of these involves a minimal change to the original code yet provides substantial parallel performance up to nearly a hundred processors. Another more ambitious project has developed a more scalable version which demonstrates acceptable performance on several hundred processors. This code is being used to study a full dimer of acetylcholinesterase in solution, involving over 130,000 atoms in the simulation.

Finally, we will mention recent work parallelizing molecular imaging codes. This is allowing electron microscope data to be reconstructed to a much greater accuracy than possible before. The computational algorithms that are widely used have novel data access patterns that pose interesting challenges for distributed-shared-memory systems. These emerging parallel supercomputer systems are expected to dominate the market in the future, and imaging algorithms provide an important new source of guiding experience that can help in making critical design decisions for novel computer architectures.

10:30 am	<b>Coffee Break</b>	IMA Lounge, Vincent Hall 502
11:00 am	<b>De Witt Sumners</b> Florida State University	Topological approaches to molecular structure

*Abstract:* Topology is a useful tool for describing and computing spatial conformation of both large and small molecules. This talk will discuss topological methods used to discriminate between stereoisomers of small molecules, and methods used to quantify entanglement of macromolecules. The mathematical methods include Monte Carlo simulation, analytic proofs, and hybrids of proof and simulation. Applications to synthetic polymers (polyethylene) and biopolymers (DNA) will be discussed.

2:00 pm	<b>Craig J. Benham</b> Mount Sinai School of Medicine	Sites of Superhelical DNA Duplex Destabilization Occur at Specific Regulatory Regions
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*Abstract:* DNA within living organisms occurs in a superhelical condition, which imposes stresses on the molecule. These stresses can destabilize the B-form duplex, causing local strand separations to occur at the sites where the thermodynamic stability is least. Theoretical methods have been developed to predict the locations and

extents of destabilization in superhelical DNA sequences [1]. The results of these analyses agree precisely with experimental determinations of the extents and locations of denatured regions, as found by nuclease digestion [2]. This allows their use to predict the destabilization properties of other sequences, on which experiments have not been performed.

These methods have been applied to the analysis of genomic sequences from a wide range of organisms [3, 4]. The sites of predicted duplex destabilizations do not occur at random, but instead are closely associated with several specific types of DNA regulatory regions. The most strongly destabilized sites occur in the 3' flanks of genes. This pattern is detected in prokaryotes, eukaryotic viruses, yeast and humans. An analysis of 26 yeast genes found that their promoter and terminal regions were destabilized, but the region encoding the primary transcript was not. This same tripartite pattern is found in rDNA sequences, which are transcribed by a different polymerase.

Origins of replication contain regions that are susceptible to stress-induced strand separation. The autonomously replicating sequences (ARSs) in the yeast genome require a destabilized site at a specific location to be active.

The third class of regulatory regions that exhibit characteristic destabilization properties are sites of DNA attachment. Scaffold attachment regions (SARs), which are sites where the chromatin fiber is attached to the chromosomal matrix, contain sites of stress-induced destabilization. The centromere regions of two yeast species (baker's yeast and fission yeast) both contain sites where the strands of the DNA duplex separate under imposed stress. It appears that the single strands within this region form hairpin structures that are involved in kinetochore binding [5].

This talk will briefly describe the techniques used to analyze duplex destabilization in superhelical DNA. A selection of predictions regarding the destabilization properties of these three classes of regulatory regions will be presented. The implications of these results concerning possible regulatory mechanisms will be considered.

The strong associations found between stress-destabilized sites and specific categories of regulatory regions suggests that the presence of such sites may be necessary for function. Experimental results support this conclusion in several specific cases. This suggests that methods to evaluate the destabilization properties of putative regulatory regions may be useful in discriminating which sites are active. The incorporation of these methods into strategies to search genomic sequences for regulatory regions will be discussed.

#### References:

- [1] C.J. Benham (1990) Theoretical Analysis of Heteropolymeric Transitions in superhelical DNA Molecules of Specified Sequence, *J. Chem. Phys.* **92**: 6294-6305.
- [2] C.J. Benham (1992) Energetics of the Strand Separation Transition in Superhelical DNA, *J. Mol. Biol.* **225**: 835-847.
- [3] C.J. Benham (1993) Sites of Predicted Stress-Induced DNA Duplex Destabilization Occur Preferentially at Regulatory Loci, *Proc. Nat'l. Acad. Sci. USA* **90**: 2999-3003.
- [4] C.J. Benham (1996) Duplex Destabilization in Superhelical DNA is Predicted to Occur at Specific Transcriptional Regulatory Regions, *J. Mol. Biol.* **255**: 425-434.
- [5] M. Tal, F. Shimron and G. Yagil (1994) Unwound Regions in Yeast Centromere IV DNA, *J. Mol. Biol.* **243**: 179-189.

3:00 pm	<b>Coffee Break</b>	IMA Lounge, Vincent Hall 502
3:30 pm	<b>Robert Manning</b> University of Maryland	Continuum Mechanics Computations of DNA Cyclization

*Abstract:* Cyclization of short DNA molecules (150-160 bp) is an excellent testing ground for continuum elastic models, in that entropic and solvent effects are minimized, so one can focus on the mechanics of DNA bending and twisting. We have computed cyclization equilibria using a combination of (1) a continuum model which includes DNA intrinsic curvature derived from experimental studies of base-pair stacking, (2) parameter continuation computations using the collocation package AUTO, (3) stability computations to determine which equilibria are local minima, and (4) visualization software tailored to the continuation computations. This combination gives a qualitative understanding of the set of equilibria as physical parameters (e.g. bend phasing, DNA length,

twist and bend stiffnesses) are varied. Continuum cyclization energies match the equilibrium energies of the base-pair-level wedge-angle model, and also agree with experimental cyclization rates.

This project represents joint work with John Maddocks, Jason Kahn, and Kathleen Rogers.

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**Friday, January 24**

**IMA Industrial Postdocs Seminar**

The seminar will meet from 1:30 pm – 4:30 pm today. The format of the seminar is:

1. Presentation of projects and problems from industry (Honeywell, Lockheed Martin and Kodak) on which the industrial postdocs are working.
2. Informal suggestions and discussion among the participants.

The seminar is directed by Avner Friedman and Walter Littman. Visitors who plan to attend are requested to inform Dr. Friedman.

The seminar meets in Vincent Hall 570

**Monday, January 27**

**Joint IMA-Math Department Special Lecture in Vincent Hall 570:**

2:30 pm	<b>Gopi Kallianpur</b> University of North Carolina	Operator-valued stochastic evolution equations and a stochastic Dyson formula
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**Math Department Seminar on Math Physics in room Vin H 570:**

3:30 pm	<b>Andrzej Daszkiewicz</b> Copernicus Univ., Poland	Some applications of moment maps in representation theory
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*Abstract:* A reductive dual pair is a pair  $(G, G')$  of subgroups of a symplectic group  $Sp(W)$ , for some real symplectic vector space  $W$ , such that each of them is equal to the centralizer or the other one and both act reductively on  $W$ . The Howe duality establishes a bijection  $\Pi \leftrightarrow \Pi'$  between certain sets of irreducible admissible representations of  $G$  and  $G'$  (or, more precisely, of their double coverings in the metaplectic group). One of the important geometric invariants of a representation  $\Pi$  of a group  $G$  is its *wave front set*  $WF(\Pi) \subseteq \mathfrak{g}^*$  ( $\mathfrak{g}$  is the Lie algebra of  $G$ ), describing the singularities of the distribution character of the representation. A conjecture of Howe says that for a "general" pair  $(\Pi, \Pi')$  of representations in Howe duality their wave front sets should be related via the moment maps  $\tau : W \rightarrow \mathfrak{g}^*$ ,  $\tau' : W \rightarrow \mathfrak{g}'^*$ . The aim of the talk is to describe my joint work with Tomasz Przebinda (University of Oklahoma) related to this conjecture.

If time permits I will say a few words about another situation in representation theory where moment maps occur naturally, namely the theory of multiplicity-free representations.

**Tuesday, January 28**

**IMA Postdoc Seminar**



In this talk I will examine the effects of several different representations for the exchange interaction on a square 2-D grid. Although the representations agree for sufficiently fine meshes, at the scale available for micromagnetic calculations they produce different results. This will be shown both analytically and by simulations testing vortex and domain wall mobility. In particular, a surprising consequence of this analysis, that grid refinements (at the aforementioned scale) actually yield inferior results, will be demonstrated.

This talk will include a brief introduction to micromagnetics, and also present some experimental images of magnetic domains captured via magnetic force microscopy (MFM).

**The seminar meets in the Seminar Room, Vincent Hall 570.**

<b>CURRENT IMA PARTICIPANTS</b>
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POSTDOCTORAL MEMBERS FOR 1996-97 PROGRAM YEAR

NAME	PREVIOUS INSTITUTION
GOBBERT, MATTHIAS	Arizona State University
LOTOTSKY, SERGEY	University of Southern California
MALIASSOV, SERGUEI	Texas A&M University
NGUYEN, BRIAN	University of Michigan
NIE, QING	Ohio State University
SARKAR, SANHITA	University of Minnesota
SUCHOMEL, BRIAN	University of Wyoming
YANG, DAOQI	Wayne State University

POSTDOCTORAL MEMBERSHIPS IN INDUSTRIAL MATHEMATICS FOR 1996-97

NAME	PREVIOUS INSTITUTION	INDUSTRIAL AFFILIATION
CHAWLA, SANJAY	University of Tennessee	Honeywell
KOURITZIN, MICHAEL	Carleton University	Lockheed Martin
LOPEZ, GILBERTO	Northwestern University	Eastman Kodak
WANG, LEI	University of Washington	Honeywell

VISITORS IN RESIDENCE (as of 12/6)

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ANDERSEN, HANS	Stanford University	JAN 19 - 24
BENHAM, CRAIG	Mount Sinai Medical Center	JAN 19 - 24
BJØRSTAD, PETTER	University of Bergen	SEP 1 - JUN 30
BRENNER, SUSANNE	University of South Carolina	JAN 13 - JUN 30
CHENEY, MARGARET	Rensselaer Polytechnic Institute	JAN 1 - JUN 30
COCKBURN, BERNARDO	University of Minnesota	SEP 1 - AUG 31
DONAHUE, MIKE	NIST	JAN 30 - 31
FRIEDMAN, AVNER	University of Minnesota	SEP 1 - AUG 31
FRIESNER, RICHARD	Columbia University	JAN 19 - 24
GULLIVER, ROBERT	Institute for Mathematics	SEP 1 - AUG 31
HABASHY, TAREK M.	Schlumberger-Doll Research	JAN 30 - 31
HEJHAL, DENNIS	University of Minnesota	SEP 1 - AUG 31
HERMANS, JAN	University of North Carolina	JAN 19 - 24
KALOS, MAL	Cornell University	JAN 19 - 24
KRUZIK, MARTIN	Czech Academy of Sciences	SEP 1 - JUN 30
LEIMKUHNER, BENEDICT	University of Kansas	JAN 19 - 29
LI, GARY	Motorola	JAN 16 - 19
LIANG, JIE	University of Illinois at Urbana	JUN 29 - 30
LITTMAN, WALTER	University of Minnesota	SEP 1 - AUG 31
LOWENGRUB, JOHN	University of Minnesota	SEP 1 - AUG 31
LUSKIN, MITCHELL	University of Minnesota	SEP 1 - AUG 31
MANNING, ROBERT S.	University of Maryland	JAN 18 - 24
MORÉ, JORGE	Argonne National Laboratories	JAN 19 - 24

PAFFENROTH, RANDY	University of Maryland	JAN 18 - 24
PARDALOS, PARNOS	University of Florida	JAN 1 - 31
PROHL, ANDREAS	Universitaet Heidelberg	SEP 1 - JUN 30
RACKNER, BARRY	Minnesota Supercomputer Center	SEP 1 - AUG 31
SCHLICK, TAMAR	New York University	JAN 14 - 24
SCOTT, RIDGWAY	University of Houston-University Park	JAN 6 - MAR 31
SELL, GEORGE	University of Minnesota	SEP 1 - AUG 31
SKEEL, ROBERT	University of Illinois - Urbana	JAN 19 - 24
SUMNERS, DEWITT	Florida State University	JAN 1 - 31
ŠVERÁK, VLADIMIR	University of Minnesota	SEP 1 - AUG 31
WILLINGER, WALTER	Bellcore	JAN 9 - 10
WU, ZHIJUN	Argonne National Laboratory	JAN 19 - 24
XIE, DEXUAN	New York University	JAN 19 - 25