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UNIVERSITY OF MINNESOTA

Supercomputing Institute

Research Bulletin

for Digital Simulation and Advanced Computation

Multi-constraint Graph Partitioning for Emerging Applications in Scientific Simulations

Algorithms that find good partitionings of highly unstructured and irregular graphs are critical for developing efficient solutions for a wide range of problems in many applications on both serial and parallel computers. Traditional graph partitioning problems focus on computing a partitioning of a graph such that each domain has an equal number of vertices, and the number of edges cut by partitioning is minimized. This graph partitioning problem is widely used for static distribution of the mesh in parallel scientific simulations, VLSI design, and many other areas. While no algorithms are known to produce verifiably optimal solutions in a reasonable amount of time, a number of multilevel algorithms have been developed recently that are able to obtain near-optimal results very quickly.

Researchers at the University of Minnesota Army High Performance Computing Research Center (AHPCRC) have been working on developing and implementing these algorithms. Professor Vipin Kumar and Assistant Professor George Karypis of the Department of Computer Science and Engineering and AHPCRC at the University of Minnesota are the principal investigators for this project.

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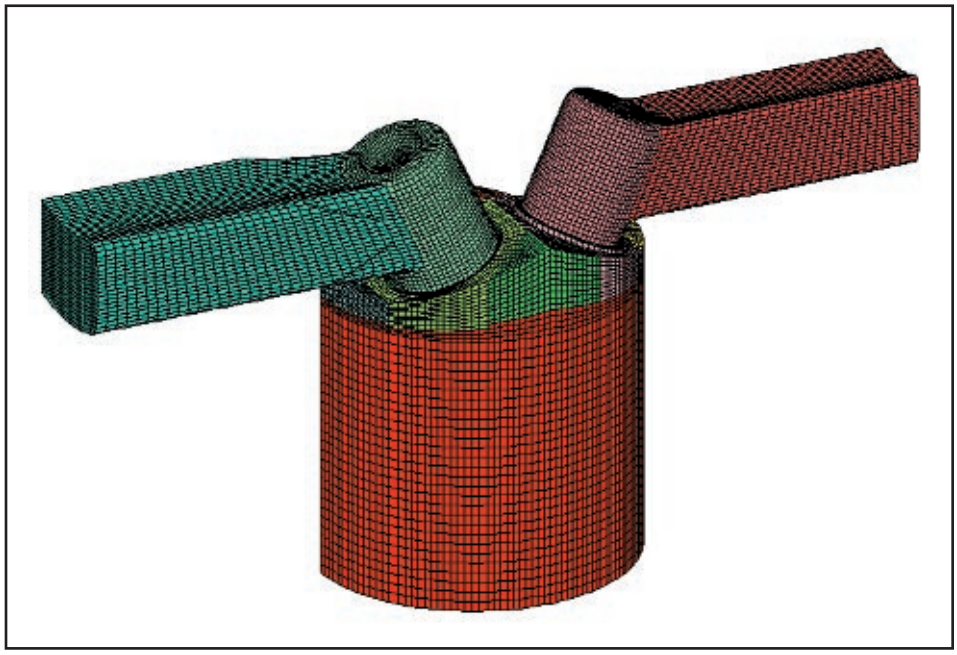
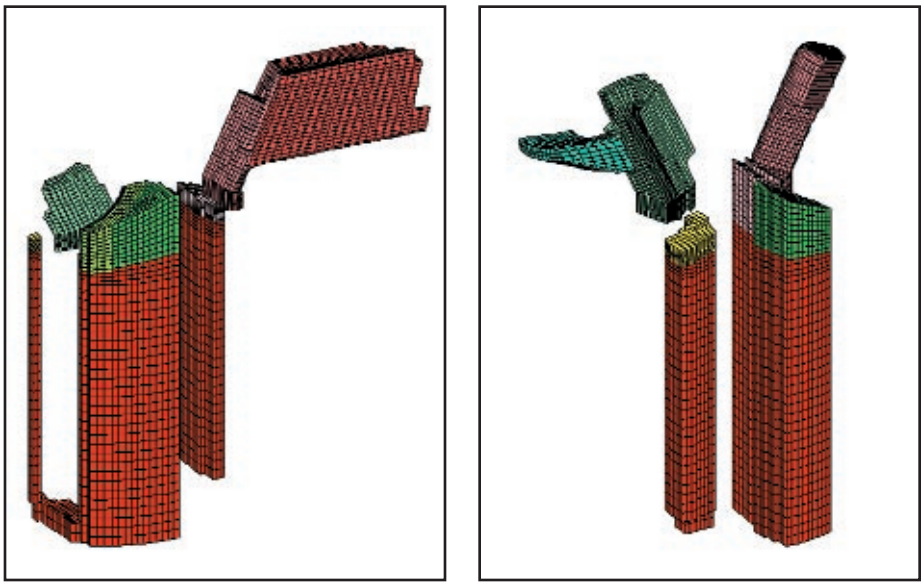


Mesh for a 6-phase automobile engine simulation. Each color represents a different computational phase. A partitioning is required in which every domain contains an equal amount of vertices of each different color. Mesh provided by Analysis and Design Application Company Limited.

Multi-constraint Graph Partitioning

Continued from page 1

Professor Kumar is a Fellow of the Supercomputing Institute. They, along with Graduate Student Researcher Kirk Schloegel of the Department of Computer Science and Engineering at the University of Minnesota, have implemented static and dynamic serial and parallel graph partitioning libraries called Metis and ParMetis. These libraries are widely used for a variety of applications in government, academia, and industry. They have been shown to be scalable to graphs with very large numbers of vertices. In fact, ParMetis is able to compute a 128-way partitioning of an eight million element three-dimensional finite element mesh in less than nine seconds on a 128-processor Cray T3D.



Two domains from an 8-way partitioning computed using the multi-constraint partitioning algorithm implemented in the Metis library. Mesh provided by Analysis and Design Application Company Limited.

Unfortunately, the traditional graph partitioning problem alone is not sufficient to model the underlying requirements of many current and emerging applications, especially in the area of high-performance scientific simulations. For example, the effective parallel solution of multi-phase computations in areas such as automobile engine design (see figures) and crash-worthiness testing requires that the partitioning algorithm simultaneously balance the computations performed during each one of the phases and minimize the various communication overheads—none of which can be accomplished by current graph models and partitioning algorithms. A number of emerging applications also require that not only computation, but also memory requirements be balanced across the processors to allow the execution of very large problems on parallel machines. These problems are better modeled by multi-constraint graph partitioning in which each vertex has multiple weights, and desired partitioning is such that sums of each of the vertex weights are balanced across all domains.

Currently, this group is developing new generalized formulations for multi-constraint graph partitioning and algorithms for solving these problems. Initial versions of these algorithms are already included in the Metis library (available at www-users.cs.umn.edu/~karypis/metis). ■

Gas Phase Nucleation of Particles during Semiconductor Processing

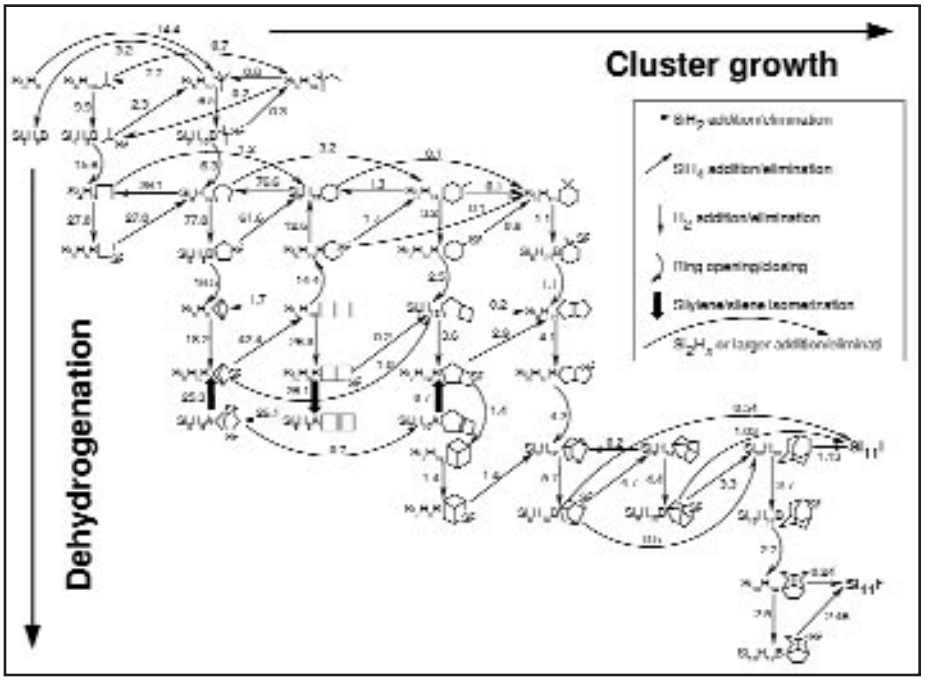
Contaminant particles are currently the major source of yield loss in the manufacture of computer chips. Particles that land on a wafer during manufacture can interrupt an electrical current path or destroy the precise planarity required for multilevel circuits. The source of these particles is not ambient dust—this is controlled effectively by clean rooms—but the actual process through which the chips are manufactured. Most particles smaller than about 100 nanometers are generated by gas phase nucleation, initiated by the same chemistries and conditions used to deposit thin films during circuit fabrication. As electronic devices become smaller, the critical size above which a particle causes 'killer' defects is also shrinking, with the critical size of these particles anticipated to reach fifty nanometers within the next few years.

Numerical models of particle nucleation and growth in semiconductor process environments are being developed by Professors Steven Girshick, Uwe Kortshagen, and Peter McMurry in the Department of Mechanical Engineering at the University of Minnesota. Professors Girshick and McMurry are Associate Fellows of the Supercomputing Institute. These investigators are working with graduate students Sandeep Nijhawan, Song-Moon Suh, Milind Mahajan, and Upendra Bhandarkar in addition to a postdoctoral research associate, Mark Swihart. This work is part of a larger effort including experimental studies that involve Professor Stephen Campbell of the Electrical and Computer Engineering Department at the University of Minnesota. The research is supported by grants from the Semiconductor Research Corporation, Advanced Silicon Materials, Inc., the National Science Foundation, and the Supercomputing Institute.

Developing these models is a challenging problem involving chemically reacting flow and/or plasmas, chemical clustering, and aerosol dynamics. Recent work has focussed on nucleation in silane, one of the most widely used process gases. For example, the figure below shows simulation results for the dominant reaction paths to particle nucleation during thermal decomposition of silane under conditions typical of the production of high-purity polysilicon rods. The silicon hydrides and reactions represent only a small fraction of the total reaction mechanism considered. The ability to conduct these simulations required substantial new development of the database of thermochemical and kinetic properties of silicon hydrides.

These clustering models are coupled to aerosol dynamics models, which allow predictions of particle growth by surface reactions, coagulation, and transport. Simulations have been conducted to study the effects of temperature, pressure, silane concentration, and carrier gas. Comparisons of these simulations with experimental results are quite encouraging.

The clustering mechanism for silane is being extended to the more complicated case of plasma-activated chemistry. In addition, more complex chemistries are being considered, such as the silane-oxygen system used for deposition of silicon oxide dielectric films.



Predicted paths to particle nucleation in silane. Numbers next to the arrows indicate net reaction rates in units of 10^{-15} mol cm^{-3} s^{-1}.

Computational Problems in Multi-Component / Multi-Phase Elastic Materials

Many structural metals—steels, aluminum alloys, and superalloys—are products of solid-state diffusional phase transformations. These transformations occur when the temperature of an alloy is abruptly lowered and a thermodynamically stable single phase separates into multiple phases at these lower temperatures. This separation, which occurs by diffusion of matter among the phases, depends on the thermodynamics of the system, the elastic fields generated by the transformation, and the surface energy of the interfaces between phases. The end result of the transformation process is the formation of a multi-phase microstructure, which is a key variable in setting the mechanical properties (stiffness, strength, toughness) of the alloy.

In many alloys (especially those used at high temperatures), there is an *in situ* transformation process called coarsening in which a dispersion of very small precipitates evolve to a system of a few very large precipitates. This coarsening process severely degrades the properties of the alloy, in some cases leading to failure. While reduction of surface energy is the overall driving force for coarsening, the process also depends strongly on the elastic properties and crystal structures of the alloy phases. By carefully choosing the alloy components, it may be possible to use the elastic properties to slow or eliminate coarsening and improve material performance over time.

Over the past several years, Professors Perry Leo of the Aerospace Engineering and Mechanics Department and John Lowengrub of the School of Mathematics at the University of Minnesota, together with collaborators Herng-Jeng Jou (Colorado School of Mines) and Qing Nie (University of Chicago), have been developing mathematical models and computational methods to predict microstructural features in alloys in two space dimensions. Professor Lowengrub is a Fellow of the Supercomputing Institute, and Professor Leo is an Associate Fellow.

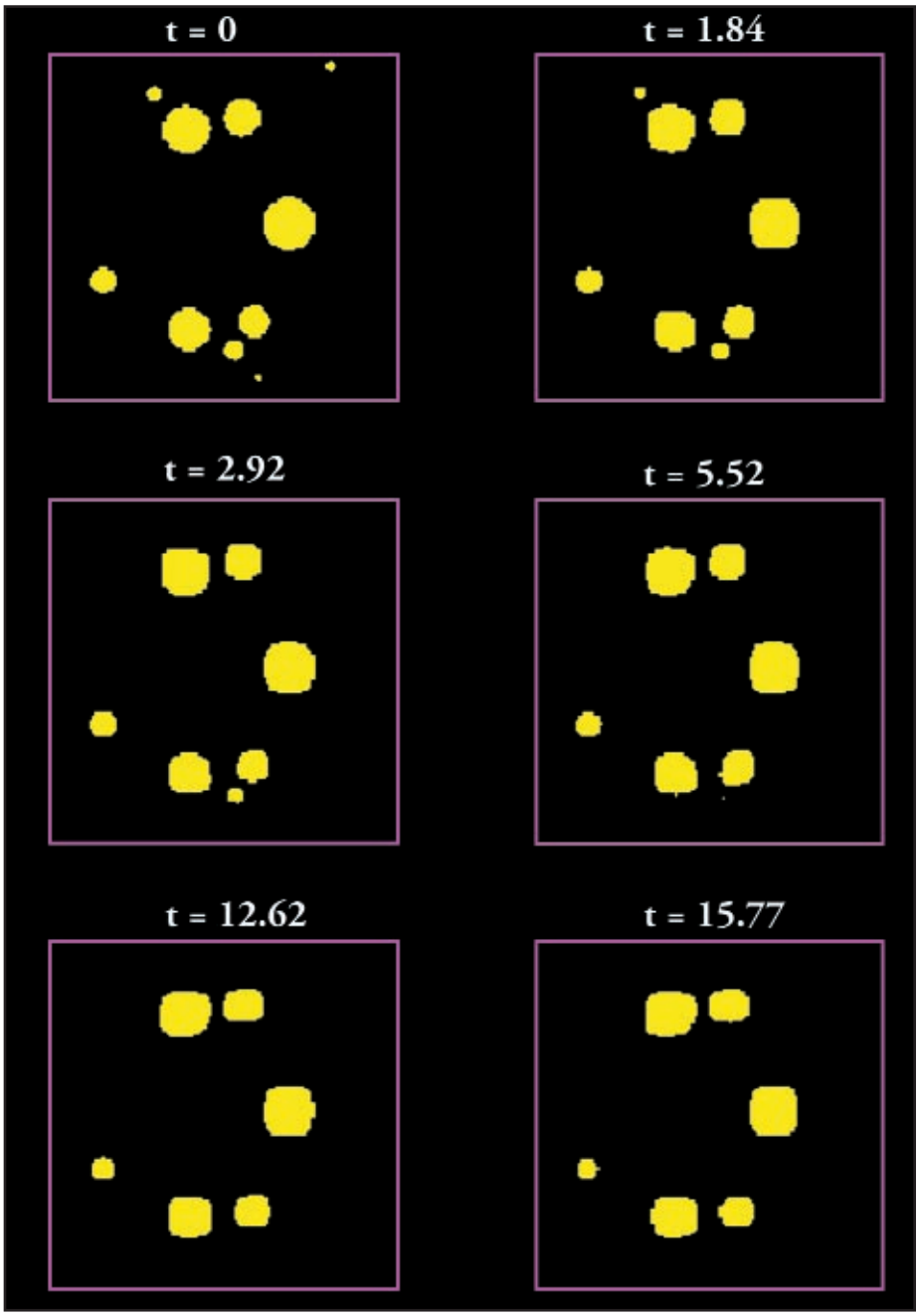


Figure 1: Evolution of 10 Ni_3Al precipitates in a *Ni* matrix.

These investigators work involves understanding and simulating the interactions among diffusion, elastic stresses, and surface energy during microstructural evolution. Their research group is the first to develop methods that incorporate elastic inhomogeneity and anisotropy in dynamic simulations.

Leo and Lowengrub's research group has focused on two types of techniques to study microstructural evolution—boundary integral methods (BIM) in which the precipitate-matrix boundaries are assumed to have zero thickness and diffuse interface methods (DIM) in which the boundaries have finite but narrow thickness. In BIM, field equations are mapped to sharp boundaries between phases, and boundary conditions are used to formulate boundary integral equations. In DIM, evolution of the smooth fields is given by a coupled set of partial differential equations.

The BIM is efficient because dimensionality of the governing equations is reduced. Furthermore, Leo, Lowengrub, and Nie have developed highly efficient and accurate algorithms using parallel computations. Efficiencies of 90% are regularly achieved. The BIM results include studies of growth shapes and coarsening shapes in elastically inhomogeneous systems using both isotropic and anisotropic elasticity. A calculation of multiparticle evolution is shown in Figure 1. Parameters appropriate to a *Ni-Al* system are chosen, with the matrix phase being essentially pure *Ni* and the precipitate phase being Ni_3-*Al*. Both phases have cubic anisotropy. The precipitates are circular at $t = 0$. As they evolve, their shapes become squarish, reflecting the underlying crystal, and they begin to align along the horizontal direction. In addition, the particles attract each other, which is shown to be a characteristic of the elastic constants used in the simulation. Such behavior may indicate that the particles eventually merge.

One drawback of BIM is that equations break down when topological changes such as merging or vanishing of precipitates occur. To compute the system in Figure 1, precipitates were simply removed when their area dropped to less than 0.1. On the other hand, while the DIM is more expensive than the BIM, the DIM is useful because it naturally handles particle merging and vanishing via a smooth transition region between phases. This is illustrated in Figure 2 where the evolution of a system of twelve precipitates in an isotropic matrix is shown. Here, a smooth coarsening evolution towards a plate-like structure is observed.

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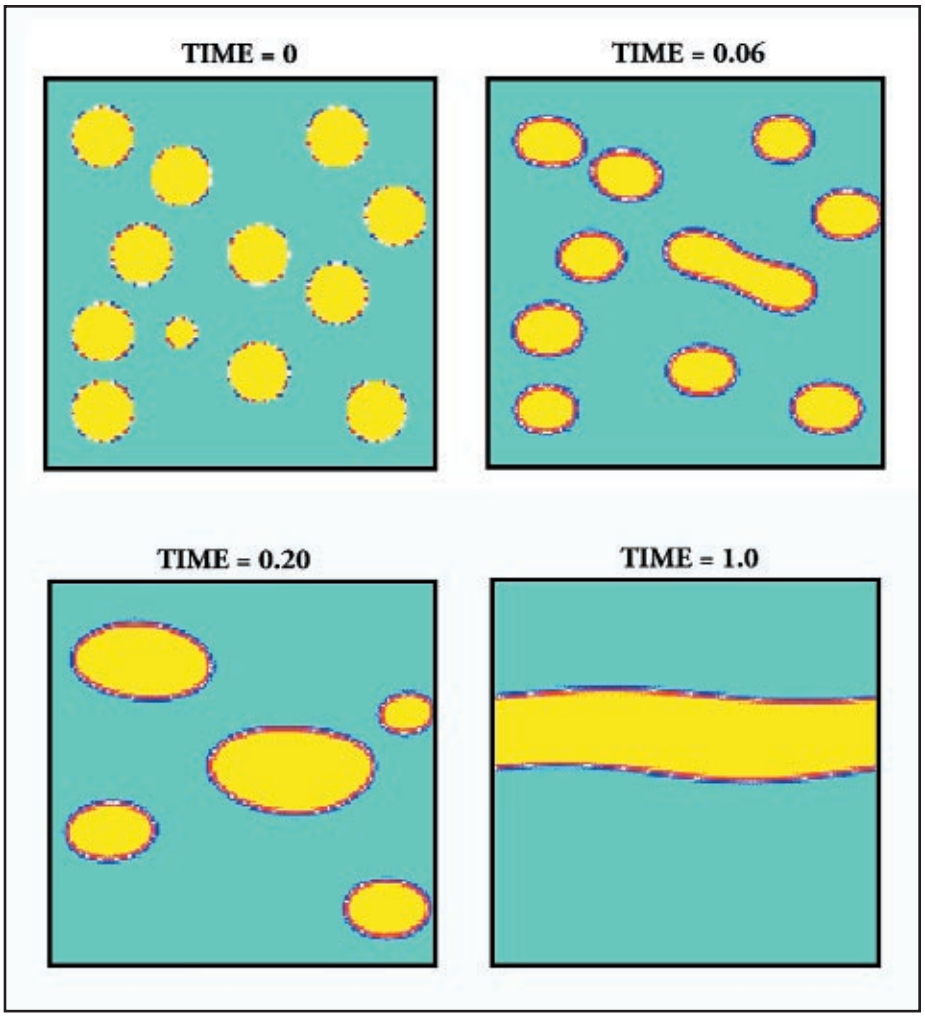

Figure 2: Evolution of 12 isotropic precipitates in an isotropic matrix. Shear modulus of precipitates is one half that of the matrix.

Estimating Hospital Quality Using a Bayesian Selection Model

Measuring the quality of care being provided to hospital patients is a vexing—albeit important—problem facing health care researchers. As hospitals are more exposed to market forces, it has become increasingly necessary to understand how competitive factors have affected the quality of hospital care provided by different types of institutions and to different types of patients. Patient discharge databases allow researchers to measure hospital-specific mortality and use these as outcome-based measures of quality. Hospitals with higher mortality (after controlling for other factors) would be found to have lower quality.

This analysis is complicated by one important fact—more severely ill patients are more likely, all else being equal, to choose higher quality hospitals. Thus, hospital-specific mortality rates will reflect both the quality of the hospital and the severity of illness of the patients. As hospital choice is correlated with severity of illness, and severity of illness cannot be perfectly observed, standard estimation techniques will give incorrect estimates of hospital-specific quality.

Professors Gautam Gowrisankaran and John Geweke of the Economics Department at the University of Minnesota and Professor Robert Town of the School of Management at the University of California in Irvine, California are developing a selection model technique to consistently estimate hospital-specific mortality in the presence of unobservable severity of illness by using geographical data from the United States Census. The basis for this estimation process is to model patient choice of hospital using distance as the principal predictor. If a hospital is drawing patients from further away than other hospitals, that hospital is attracting patients with relatively high severity of illness. In this way, the use of geographical measures allow a separation of the two confounding effects, severity of illness and hospital quality, that both affect hospital mortality. This simple insight is then used in Bayesian econometrics to develop accurate estimates and predictions as to hospital quality.

Preliminary results indicate that selection is an important determinant of hospital mortality, and controlling for selection yields substantially different predictions as to hospital quality. For instance, the estimated distribution of predicted mortality rates is compared for a randomly selected patient if that patient were to seek treatment at two different hospitals, Los Angeles County / University of Southern California (USC) Medical Center (a large, public teaching hospital located in East Los Angeles) and the University of California–Los Angeles (UCLA) Medical Center (a well-regarded, private teaching hospital located in West Los Angeles). Figure 1 shows the results controlling for unobserved patient selection while Figure 2 shows the results with standard methods. Points above the 45° line indicate a lower estimated mortality (higher estimated quality) for UCLA. One can see from Figure 1 that, by controlling for selection, UCLA Medical Center is revealed to be of higher quality than LA County / USC Medical Center. In contrast, standard methods from Figure 2 give exactly the opposite prediction. A

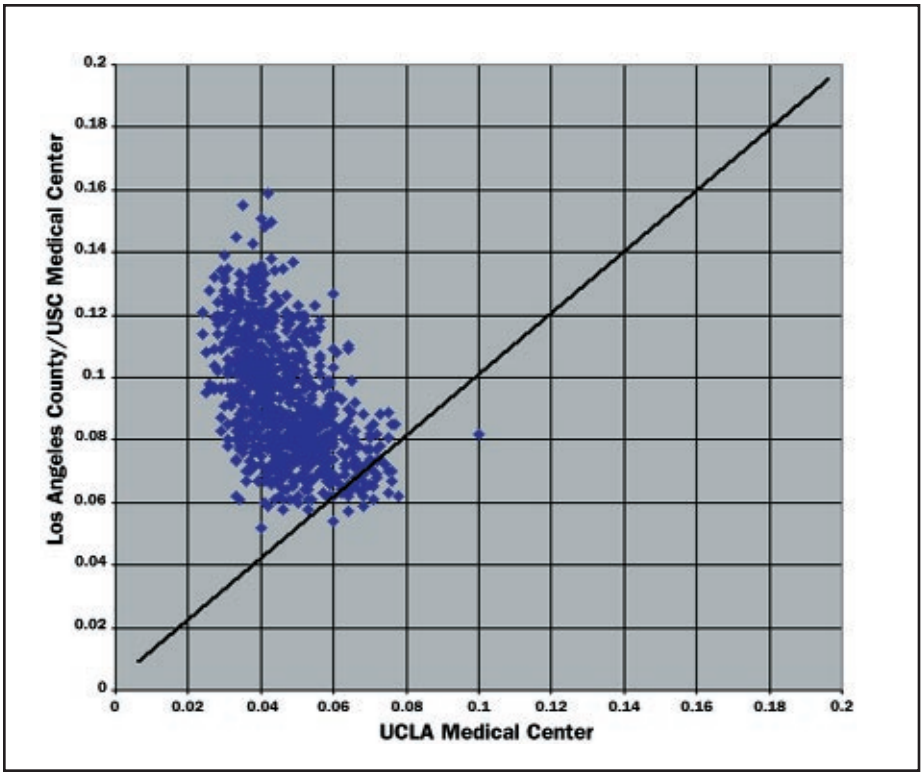

Figure 1: Probability of death by hospital using the Bayesian selection model.

long-run goal is to further explore the determinants of hospital quality by ownership type and to examine how competition and costs affect quality.

Because of the large size of the data set (20 thousand patients per year for 4 years and 100 hospitals just in Los Angeles County), these methods are very computationally intensive. Furthermore, the Bayesian estimates are computed using an iterative process, with approximately 10,000 iterations required for convergence. Using a Sun UltraSparc II 300 MHz computer, these researchers were able to compute each iteration in approximately 30 minutes. Using the IBM SP supercomputer and ESSL library routines for matrix multiplication, these researchers computed the algorithm in approximately 6 minutes per iteration. They then rewrote the code to take advantage of the parallel architecture of the IBM SP making use of the Message Passing Interface paradigm. The use of parallel algorithms resulted in substantial speed increases that made the algorithm feasible. For instance, the algorithm takes 100 seconds per iteration with 4 processors, 60 seconds per iteration with 8 processors, 40 seconds per iteration with 16 processors, and 33 seconds per iteration with 20 nodes.

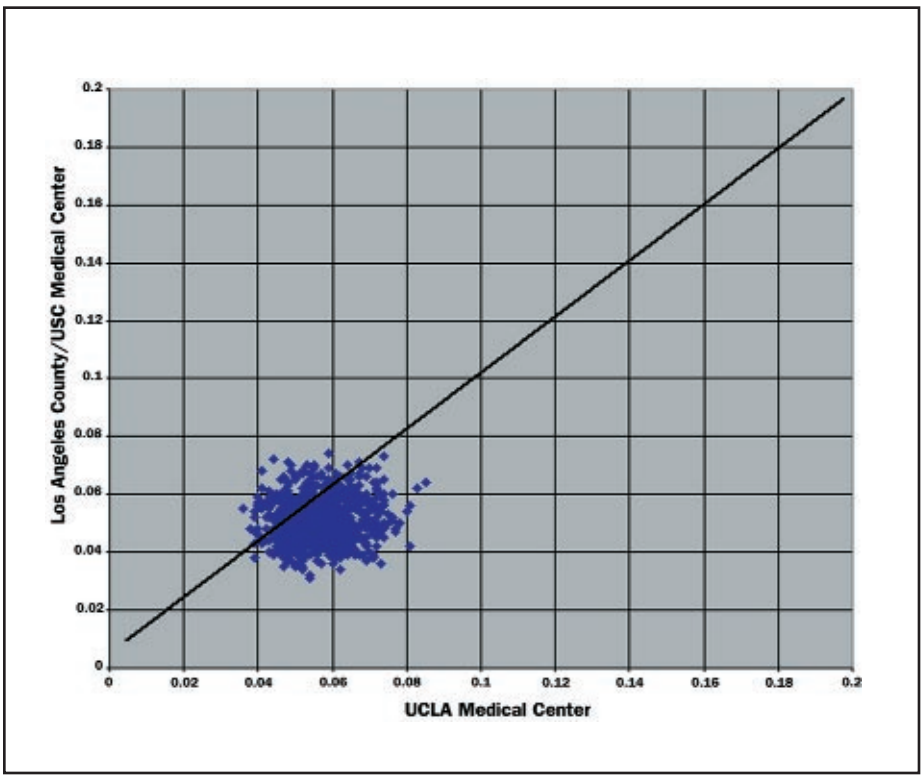

Figure 2: Probability of death by hospital using standard (non-selection) methods.

Multi-Component / Multi-Phase Materials

Continued from page 5

Leo and Lowengrub's research group is continuing to refine and enhance their methods to perform successively more realistic simulations of microstructure evolution. The group intends to study the coarsening statistics of systems of many precipitates in the future, developing three-dimensional models and including non-equilibrium effects such as interface kinetics in systems where the precipitate and matrix have very different crystal structures. By accurately simulating the formation of microstructure in alloys, Leo and Lowengrub hope to eventually be able to provide metallurgists with a prescription for generating alloys with desirable material properties.

Future Symposium

1999 International Conference on Preconditioning Techniques for Large Sparse Matrix Problems in Industrial Applications

June 10–12, 1999

This conference will address complex issues related to the solution of general sparse linear systems of equations in real applications, or specifically in an industrial setting. It is often observed that the issues of interest to industrial users of linear systems solution software are fairly different from those the academic community is focussed on. In an industrial context, improving robustness is more important than finding a method to gain speed. Memory usage is also an important consideration seldom accounted for in academic research on sparse solvers. Finally, linear systems solved in applications are almost always part of some nonlinear iteration (e.g., Newton) or optimization loop, and it is important to consider the coupling between the linear and nonlinear parts instead of focussing on the linear system alone.

More Information

Additional information regarding the conference, presenting a poster paper, travel support, and registering for the conference is available on the World Wide Web at:

www2.msi.umn.edu/Symposia/sparse99

by sending email to:

sparse99@msi.umn.edu

or by contacting Michael Olesen, the Conference Administrator, at:

(612) 624-1356

Poster Papers

The program committee has issued a call for poster papers related to the conference's themes and motivations. The deadline for submitting poster paper abstracts is April 22, 1999. Poster paper abstracts should be submitted to:

Sparse-99
Supercomputing Institute
University of Minnesota
1200 Washington Avenue South
Minneapolis, MN 55415

or, abstracts can be submitted electronically (postscript) to:

sparse99@msi.umn.edu

The maximum length of the abstract should be one (1) page.

Speakers and Topics

Raymond Honfu Chan, Chinese University of Hong Kong, Hong Kong
Preconditioning Techniques for Toeplitz Systems and their Applications in High-Resolution Image Reconstruction

Edmond Chow, Lawrence Livermore National Laboratory
Parallel Preconditioning for Multiphysics Simulations with Sliding Interfaces

Howard C. Elman, University of Maryland
The Schur Complement and Preconditioners for Saddle Point Problems

Charbel Farhat, University of Colorado at Boulder
Recent Advances in the FETI Method for Structural Mechanics and Acoustic Scattering Problems

Peter A. Forsyth, University of Waterloo, Canada
Iterative Methods for Multi-factor Option Pricing

David Keyes, NASA Langley Research Center
Newton-Krylov Methods with Multilevel Preconditioning: Algorithm-Architecture Trade-offs in the Number of Levels

John G. Lewis and **Daniel J. Pierce**, Boeing Computer Services
Iterative Solution of Sparse Symmetric Linear Systems from Interior Point Methods

Maya Neytcheva, University of Nijimegen, The Netherlands
Fully Parallel Interface Domain Decomposition Method for Finite Element Elliptic Problems

Willy H.A. Schilders, Philips Research Laboratories, The Netherlands and
Henk A. van der Vorst, Utrecht University, The Netherlands
Preconditioning Techniques for Indefinite Linear Systems with Applications to Circuit Simulation

Justin Wan, Stanford University
Interface Preserving Coarsening and Energy-Minimizing Interpolation Multigrid Methods for Discontinuous Coefficient PDEs

First Annual University of Minnesota Computational Neuroscience Symposium

October 7–8, 1999

The Computational Neuroscience Program of the University of Minnesota, in conjunction with the Department of Neuroscience, the Graduate Programs in Scientific Computation and Neuroscience, and the Supercomputing Institute for Digital Simulation and Advanced Computation, will host a symposium on computational neuroscience on October 7 and 8 at the University of Minnesota campus. Topics include molecular mechanisms in ion channels, signal transduction, neurotransmission and receptors, computational models of vistibular and oculomotor control, robotics and computer vision, and neural network models.

Speakers and Topics

Dora Angelaki, Washington University School of Medicine
Coding of Movement in Inertial Space: Computational Problems and Neuronal Strategies

Andrew Barto, University of Massachusetts
Learning to Reach via Corrective Movements: A Neural Model

Stephen Cannon, Harvard University
Chaotic Consequences of Sodium Channel Mutations that Disrupt Inactivation

Henrietta Galiana, McGill University
The Role of Central Topology in Sensory Fusion for Oculomotor Control

Gregory Hager, Yale University
To be announced

Mitsuo Kawato, Advanced Telecommunications Research Institute, Japan
Cerebellar Internal Models for Robotics and Cognition

Tommy Liljefors, Royal Danish School of Pharmacy, Denmark
Computational Studies of Molecular Properties of Neurotransmitter Receptor Ligands in relation to their Receptor Binding

Steven Lisberger, University of California–San Francisco
How Visual Motion Signals for Pursuit are Represented in and Decoded from the Cortical Motion Areas

Mark Sansom, Oxford University, England
Simulation Studies of K^+ channels

Laurence Trussell, University of Wisconsin–Madison
The Dynamics of Transmitter Release and its Role in Shaping Neural Responses

Harel Weinstein, Mt. Sinai School of Medicine
Computational Experiments Reveal Molecular Mechanisms in Signal Transduction by Membrane Proteins

Program Committee

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Vipin Kumar, Department of Computer Science and Engineering, Co-Chair
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Apostolos Georgopoulos, Department of Neuroscience
Daniel Kersten, Department of Psychology
Robert Miller, Department of Physiology
Nikolaos Papanikolopoulos, Department of Computer Science and Engineering
John Soechting, Department of Neuroscience
Jaideep Srivastava, Department of Computer Science and Engineering
David Thomas, Department of Biochemistry, Molecular Biology, and Biophysics
Lawrence Wackett, Department of Biochemistry, Molecular Biology, and Biophysics
George Wilcox, Department of Pharmacology

More Information

More information is available on the World Wide Web at:

www.compneuro.umn.edu/symposia.html

or by sending email to:

clinton@compneuro.umn.edu

Colloquium Series

Computational Biological Sciences Colloquium Series

A Biological Problem Viewed Through the Lens of Mathematics: Pattern Formation and Morphogenesis in Early Development

Professor Hans G. Othmer
Department of Mathematics
University of Utah
Salt Lake City, Utah

How does the zebra get its stripes and the leopard its spots? Why do we have five digits on our hands and how do they come to be arranged properly? These are questions of how pattern is formed in early development, questions that have fascinated experimentalists and theoreticians for at least a hundred years. Molecular biologists have made enormous strides in understanding the signals that control gene expression, but how are the signals controlled? How do cells in a developing system 'know' where they should go and what they should do when they get there? In this seminar, Professor Othmer showed how mathematical models and computational experiments using these models shed light on some of these questions.

Professor Othmer discussed two major aspects of pattern formation and morphogenesis. The first dealt with how cells integrate the signals they detect, how they move in response to these signals, and how the microscopic behavior of individuals can be incorporated into macroscopic continuum descriptions of cell populations. A reinforced random walk and continuum limits were discussed, and Professor Othmer showed how a velocity-jump stochastic process leads to a Boltzmann-like transport equation. He went on to show how classical chemotaxis equations are obtained from this process. The second aspect dealt with the interaction of growth and pattern in a developing system. A model for vertebrate limb formation based on a fluid mechanical description of tissue was discussed, and a numerical method for treating the free boundary problem that arises in the model was demonstrated. This model can provide experimentalists with new insights into the interaction between growth, cell-cell signaling, and pattern formation in the developing limb.

Hans G. Othmer

Crumpling a Rope: From Chain Collapse Phase Transition to Protein Folding and DNA Knots

Professor Alexander Yulij Grosberg
Department of Physics and Center for Materials Science and Engineering
Massachusetts Institute of Technology
Cambridge, Massachusetts

Major biopolymers of DNA, RNA, and proteins function in the living cell in the form of compact condensed globules. From the perspective of physics, polymer condensation, or coil-globule transition, is one of the most fundamental phenomena in polymers. For simple polymers, thermodynamics of transition is well understood, but kinetics remains a challenge. For biopolymers, since they carry biologically important information, dramatically new phenomena arise. In the case of DNA, topology of knots presents a challenge for theoretical understanding. In the case of proteins, quenched but not random sequence of monomers controls thermodynamics and kinetics of reliable folding into a unique spatial structure.

This field is experiencing a very fast development. In this seminar, the review of basic concepts was complemented by a discussion of some recent achievements.

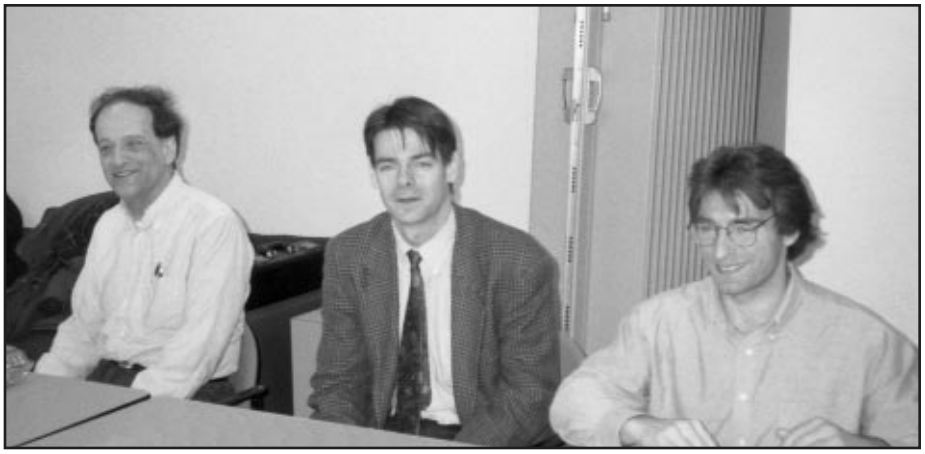
Alexander Yulij Grosberg

Statistical Mechanics Methodology for Treating Flexibility in Peptides and Proteins

Professor Hagai Meirovitch
Supercomputer Computations
Research Institute
Florida State University
Tallahassee, Florida

Conformational flexibility plays an important role in protein-protein and protein-ligand recognition. However, analysis of nuclear magnetic resonance (NMR) and X-ray data of flexible peptides and segments of proteins is difficult. A new methodology has been developed for treating flexibility based on statistical mechanics consideration; it includes new techniques for conformational search, methods for calculating the entropy and the free energy, and a novel way to parameterize solvation models. This methodology was described in Professor Meirovitch's seminar, and its potential application to problems in structural biology, drug design, and the genome project was also discussed.

Hagai Meirovitch



Professor Benoit Roux (center) with Professor Oriol Valls (left) of the School of Physics and Astronomy and Professor Darrin York (right) of the Department of Chemistry at the University of Minnesota at a lunch prior to Professor Roux's talk.

The Environment of Biomolecules: Atomic and Mean-Field Models

Professor Benoit Roux
Departments of Physics and
Chemistry
University of Montreal
Montreal, Canada

The activity of proteins and enzymes is largely influenced by the properties of the very complex environments in which they have to function. Soluble proteins function in bulk aqueous solutions. In contrast, membrane proteins function in a partly ordered, partly disordered, liquid crystalline bilayer of phospholipids. Bulk solutions, membranes, and detergent micelles are all different environments whose properties must be well-characterized at the microscopic level in order to fully understand the function of biomolecules. Computer simulations based on atomic models in which a large number of molecules are treated explicitly represent one of the most detailed approaches to studying the structure and dynamics of biological systems. Nevertheless, a significant computational cost is associated with the large number of molecules required to construct a valid microscopic model of membrane-protein systems. Furthermore, computer simulations are not exempt from serious problems. For example, particular difficulties are encountered in calculating important quantities associated with membrane functions such as the Nernst membrane potential due to the large statistical errors. Partly because of these problems, it is desirable to develop different approaches in which the influence of the membrane is incorporated implicitly. Recent developments and applications of molecular dynamics simulations, continuum electrostatics, statistical mechanical integral equations, and mean-field models were described in Professor Roux's talk.

Cognitive Neuroscience Colloquium Series

Linking Human Brain Activity with Perceptual Performance using Functional Magnetic Resonance Imaging

Professor David Heeger
Department of Psychology
Stanford University
Stanford, California

Dr. Paul Schrater (left) of the Psychology Department at the University of Minnesota, Professor David Heeger (center) of the Psychology Department at Stanford University, and host Professor Daniel Kersten (right) of the Psychology Department at the University of Minnesota talk prior to Professor Heeger's seminar.

The main focus of research in Professor David Heeger's laboratory is the use of functional magnetic resonance imaging (fMRI) to quantitatively investigate the relationship between brain and behavior. In this seminar, Professor Heeger presented results from three separate studies.

In the first study presented, perceptual studies suggested that visual motion perception was mediated by opponent mechanisms believed to correspond to mutually suppressive populations of neurons sensitive to motions in opposite directions. Strong motion opponency was found in a secondary visual cortical area known as the human MT complex (MT+). These results provided the clearest evidence to date that direction selective signals underly human MT+ responses, and neuronal signals in human MT+ support visual motion perception.

In the second study, Professor Heeger tested whether brain activity in primary visual cortex (V1) might be modulated by attention. In the experiments, subjects fixated the center of a display while performing a visual discrimination task on either the right or the left (without moving their eyes). Stimuli on the right were processed by neurons in the left hemisphere and vice versa. The results clearly demonstrated that V1 neural activity could be modulated by attention; activity modulated out of phase in the two hemispheres as attention shifted back and forth.

The third study was designed to test the controversial hypothesis that dyslexia involves a deficit in a specific visual pathway, the magnocellular (M) pathway, from the eye to the brain. Professor Heeger found a strong three-way correlation between individual differences in: (i) M pathway brain activity in areas V1 and MT+, (ii) reading performance, and (iii) performance in a motion discrimination task that depends on M pathway integrity. Subjects with greater fMRI activity were faster readers and better performers in the motion discrimination task.

Special Seminars

Special Seminars from Silicon Graphics Inc.

Two computational scientists from Silicon Graphics Inc., (SGI) came to the Institute to present seminars on topics related to the Origin 2000 supercomputer.

Ilene Carpenter, Environmental Applications Analyst from SGI, provided University researchers with practical information for porting codes from the Cray T3E and Cray parallel vector processing systems to the Origin platform. The seminar described software and hardware differences that applications analysts need to be aware of as they migrate codes. Issues discussed included data sizes, compiler and linker options, I/O libraries, parallel performance, binary data conversion, and Message Passing Interface data type conversion.

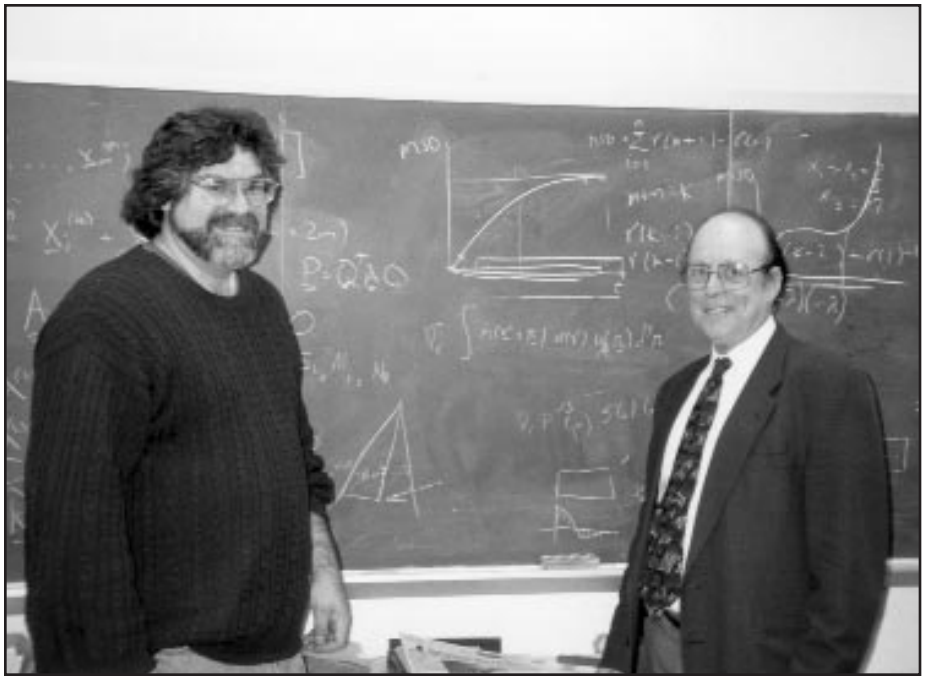
Charles Grassl, Senior Programmer Analyst from SGI, presented University researchers with a tutorial covering programming and optimization for an SGI Origin 2000 computer system. The Origin programming environment was compared and contrasted with that of Cray vector and parallel systems. The tutorial included an overview of the Origin 2000 system's macro architecture and the architecture of the MIPS R10000 microprocessor used for the processing elements. Specific optimization for single processing units were covered. Parallel programming with respect to both shared memory (directive based) and distributed memory (message passing) was also discussed.

Ilene Carpenter, Environmental Applications Analyst from Silicon Graphics, Inc., prepares for her seminar.

Charles Grassl, Senior Programmer Analyst from Silicon Graphics, Inc., speaks on the SGI Origin 2000 computer system.

Visitors

Bill Pulleyblank (right), Director of Mathematical Sciences, IBM Research, recently visited the Supercomputing Institute to discuss the Institute's research programs, IBM's plans for supercomputing, and to explore areas for further collaboration. Pictured with Dr. Pulleyblank are Pat Carey (left), Consulting Client Representative for IBM, and Donald Truhlar (center), Supercomputing Institute Director.



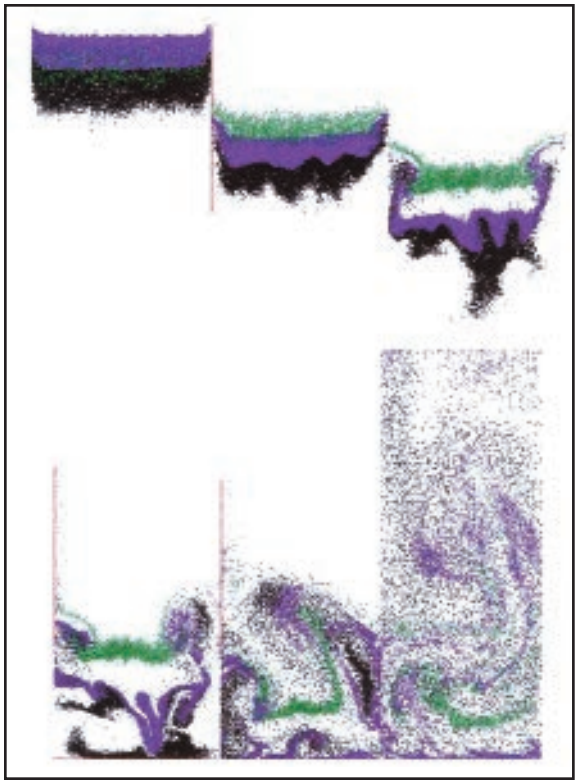
Mark Schure (left), industrial fellow for the Center for Interfacial Engineering (CIE) and Research Fellow in the Computational Chemistry group for the Rohm and Haas Company, Philadelphia, Pennsylvania and H. Ted Davis (right), Dean of the Institute of Technology, talk about lattice-Boltzmann techniques being used at CIE to simulate chromatographic separation in packed beds. The fellowship is allowing Mark to do research using parallel processing techniques on machines such as the IBM SP.

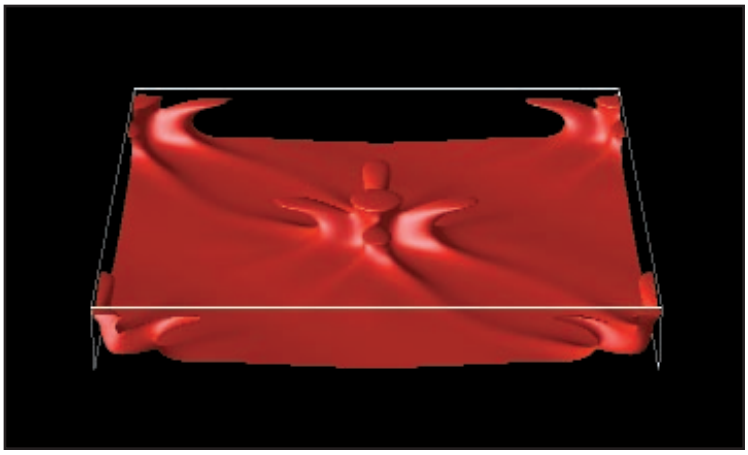
Tim Ward (left), Minneapolis Branch Manager of Silicon Graphics Inc., and Derek Robb (center), Chief Scientist of Silicon Graphics Inc., Accelerated Strategic Computing Initiative Program, met with Donald Truhlar (right), Supercomputing Institute Director, to discuss Silicon Graphics' technology plans and their involvement in the United States Department of Energy's Accelerated Strategic Computing Initiative (ASCI) program.

Students from St. Cloud, Minnesota visited the Supercomputing Institute as part of a two-year program in networking. The program, sponsored by Cisco Systems, is teaching these students valuable skills that will allow them to either enter the work force straight from high school or be well prepared for pursuing a computer science degree. While at the Institute, the students toured the supercomputing facilities and were given the opportunity to meet and talk with the Supercomputing Institute's Network Administrator, Asish Dash, who showed them how the networking and routing at the Supercomputing Institute is set up and administered.

Professor David Yuen's research team at the Supercomputing Institute added two major contributors recently when Dr. Witold Dzwinel from the Computer Science Department of the Mining and Metallurgy Institute in Krakow, Poland and Mr. Fabien Dubuffet, a graduate student from the French Space Agency in Toulouse, France came to visit. Professor Yuen (left), Dr. Dzwinel (center), and Mr. Dubuffet (right) worked on a number of geological simulations and issues.

Dr. Dzwinel worked on multi-phase flow using molecular dynamics and dissipative particle dynamics. Fabien Dubuffet worked on three-dimensional convection with variable thermal conductivity using finite-difference methods. Results from these researchers' work are shown below.

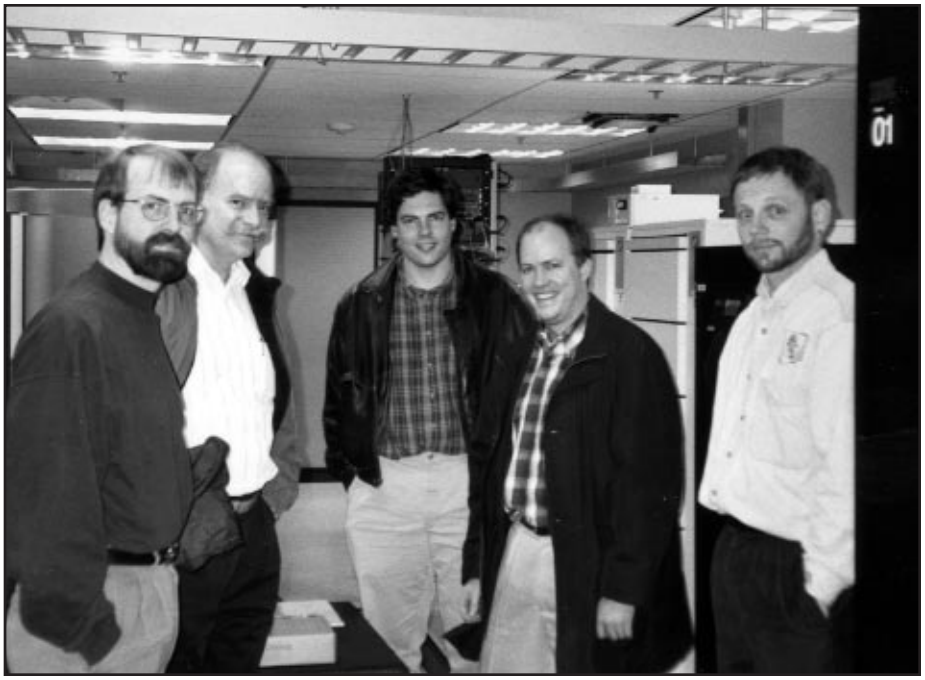




Dr. Dzwinel's work (left) shows interface layer dynamics for mixing driven by sedimentation in liquid. All six stages (three on top and three on the bottom) represent particle system after following $500 \times \Delta t$ timesteps ($\Delta t = 1$). Mr. Dubuffet's work (above) shows that at intermediate Rayleigh number convection, there is a strong nonlinear interaction between the radiative heat transfer and the convective heat transport. The tree-like plume in the middle resembles the plume detected recently under Iceland by researchers at Utrecht University in The Netherlands.

Einar Rustad (left), Vice President of Operations at SCALI Affordable Supercomputing in Skjetten, Norway, Max Tiede, Program Manager of Systems & International Programs for Lockheed Martin in St. Paul, Minnesota, Sjur Fjellbirkeland, Administrative Director for SCALI Affordable Supercomputing, and Bob Sicafuse, Manager for Business Development for Lockheed Martin (far right) met with Donald Truhlar, Supercomputing Institute Director, and Michael Olesen, Supercomputing Institute Research Programs Administrator, to discuss high-performance computing resources offered by SCALI Affordable Supercomputing.

Tom Ruwart, Assistant Director for the Laboratory for Computational Science and Engineering (LCSE)(left), Professor Paul Woodward, Director for the LCSE, and Bill Humphrey and John Reynders from the Advanced Computing Laboratory at Los Alamos National Laboratory in Los Alamos, New Mexico are looking at the supercomputers at the Institute with Barry Schaudt (far right), Manager of Systems and Operations at the Supercomputing Institute.



Supercomputing ‘98

The Supercomputing Institute was one of three partners participating in the IBM booth at Supercomputing ‘98 in Orlando, Florida, the other two being the Maui High-Performance Computing Center and PDC (a high-performance computing research center in Sweden). Tom Cortese (left), a researcher working with Professor David Yuen, Geology and Geophysics Department at the University of Minnesota, with Birali Runesha (right) of the Supercomputing Institute's User Support Staff are pictured in front of the live demonstration showing how pv3, an interactive parallel visualization program developed by Kirk Jordan of IBM, interfaces with three-dimensional mantle convection cores. The demonstration was done by co-processing, a process by which data was visualized at the same time it was being calculated. Both visualizations and calculations were done on-site by an IBM SP supercomputer with NightHawk processors.

Research Reports

Names of University of Minnesota principal investigators appear in bold type.

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A. Aguiar and **R. Fosdick**

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° 98/206, December 1998
Structural Characterization of Two Synthetic Catalysts based on Adipocyte Lipid-Binding Protein
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Crystal Structures of Native and Recombinant Yeast Fumarase
T.M. Weaver, M. Lees, V. Zaitsev, I. Zaitseva, E. Duke, P. Lindley, S. McSweeny, A. Svensson, J. Keruchenko, I. Keruchenko, K. Gladilin, and **L.J. Banaszak**

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Structures of Five Mutants of Toxic Shock Syndrome Toxin-1 with Reduced Biological Activity
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The Effect of Substrate Temperature on the Properties of Nanostructured Silicon Carbide Films Deposited by Hypersonic Plasma Particle Deposition
J. Blum, N. Tymiak, A. Neuman, Z. Wong, N.P. Rao, **S.L. Girshick**, **W.W. Gerberich**, **P.H. McMurry**, and **J. Heberlein**

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Thermal Plasma Deposition of Nanostructured Films
A. Neuman, J. Blum, N. Tymiak, Z. Wong, N.P. Rao, **W.W. Gerberich**, **P.H. McMurry**, **J. Heberlein**, and **S.L. Girshick**

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Sol-Gel Polycondensation Kinetic Modeling: Methylethoxysilanes
S.E. Rankin, **C.W. Macosko**, and **A.V. McCormick**

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J. Li, T. Zhu, G.D. Hawkins, P. Winget, D.A. Liotard, **C.J. Cramer**, and **D.G. Truhlar**

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