Supercomputing Institute Research Bulletin online
Newsletter of the University of Minnesota Supercomputing Institute

Supercomputing Institute Research Scholars

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The Supercomputing Institute is pleased to announce the appointment of five research scholars for 1998-99. Research scholars are research associates who work closely with Supercomputing Institute principal investigators.

Aditya Kumar is working with Professor Prodromos Daoutidis of the Chemical Engineering and Materials Science Department on designing and evaluating control schemes for entire chemical plants consisting of networks of chemical reactors and separation units with recycle streams. A systematic framework for plant-wide controller design is being developed. This framework uses a multi-time-scale analysis and the design of separate non-linear controllers to control characterization of slow dynamics of a plant core and fast dynamics of individual process units. This control scheme is being tested in real industrial plants through dynamic simulations of detailed plant models. Aditya received his Ph.D. in Chemical Engineering from the University of Minnesota in Minneapolis, Minnesota.

Jiabo Li, a Physical Chemistry Ph.D. from Jilin University in China, is working with Professors Christopher Cramer and Donald Truhlar of the Chemistry Department to create a universal solvation model for the computation of solvent effects on absorption and emission spectra of organic molecules. The model is universal in that it is applicable to water and all organic solvents. The model accounts for different time scales involved in response of the solvent to a newly created excited electronic state of a solute molecule, and it provides a fundamental framework for computer-aided design of photosensitive dyes. This fundamental research is supported in part by a grant from Kodak, an industrial partner. To facilitate technology transfer, a preliminary version of the model was coded into the AMSOL software package, which is in wide use for such computations on ground states. Since then, it has been coded into GAUSSIAN and GAMESS, and current work is centered on the ZINDO package. If time permits, the model will be extended to permit analysis of nonequilibrium solvation effects on chemical reaction dynamics.

Bijaya Bahadur Karki received his Ph.D. in Condensed Matter Physics from the University of Edinburgh in Edinburgh, Scotland. He is working with Professor Renata Wentzcovitch of the Chemical Engineering and Materials Science Department on performing first-principles computer simulations of high-temperature behavior for structural and elastic properties of the silicate and oxide minerals, generally considered the major consituents of the Earth's lower mantle. The methodology is based on variable-cell-shape molecular dynamics within the pseudopotential and local density approximations. Performing finite-temperature simulations requires improvement of numerical algorithms in the existing codes. In extending previous high-pressure studies of these materials, Bijaya is providing a firm theoretical basis for the physics and chemistry of the lower mantle, its composition and dynamics, and possible causes of the seismic reflectors in it.

Udo Gieseler, who received his Ph.D. in Theoretical Astrophysics from the Max-Plank-Institut für Kernphysik in Heidelberg, Germany, is working with Professor Thomas Jones of the Astronomy Department. Professor Jones' group is carrying out numerical simulations of extremely high-energy

particle production in astrophysical gas-dynamical and magnetogas-dynamical flows. Particle acceleration is a very rich subject, both in terms of basic physics and also with regard to astrophysical applications. It involves preferential transfer of much of the dynamical, flow energy into a small population of ions. Not only does this lead to a distinctive, high-energy particle population that can be observed indirectly and even directly at earth, but the acceleration and the feedback from the cosmic rays substantially modify the flows themselves in vital ways. Udo has been concentrating on the fundamental problem of injection of nonthermal particles from the thermal plasma at strong shocks. This work contributes to the development of a new class of methods that use adaptive mesh refinement and discontinuity tracking, which should enable the modeling of these physics phenomena at an unprecedented level of detail.

Masha Sosonkina-Driver is working with Professor Yousef Saad of the Computer Science and Engineering Department on developing high-performance iterative techniques for solving general sparse linear systems of equations. Masha received her Ph.D. in Computer Science and Applications from Virginia Tech in Blacksburg, Virginia. As parallel iterative methods are becoming commonplace in many fields of science and engineering, robustness and scalability of standard iterative solvers are becoming an issue. Masha is investigating and implementing a class of preconditioners that have advantages similar to robustness and scalability multigrid techniques. These methods are at the cross point between multigrid methods, domain decomposition, and incomplete LU factorizations. She is also investigating methods for retrofitting information on physical problems to compute effective incomplete LU factorizations.

Research Scholarships are awarded in response to nominations and matching funds provided by a University of Minnesota faculty member. Persons interested in a Research Scholarship in 1998-99 should contact a Supercomputing Institute Principal Investigator in their field to discuss the possibility of nomination and cosponsorship. The deadline for nominations is January 15, 1998, so it is well advised for preliminary discussions to begin this fall.

Supercomputing Institute's New Resources

This summer, the Supercomputing Institute made a transition from purchasing supercomputing services from a resource provider to directly managing and operating the major supercomputing resources it provides to the University of Minnesota research community. The primary high-performance computing research tool for the Supercomputing Institute is the 256-processor IBM SP with 192 GB of memory. This machine features the latest Symmetric Multi-Processor technology and is built with the same nodes as those that power the Department of Energy's Accelerated Strategic Computing Initiative (ASCI) project.

256-processor IBM SP supercomputer housed at the Supercomputing Institute.

The IBM SP supercomputer is a 64-node machine with four 332 MHz 604e processors and 3 GB of memory on each node. This machine is twice the size of the one used in the "Deep Blue" chess match. An additional terabyte and a half of IBM SSA disk and an IBM 3575 Tape Library are also attached.

In addition to the 256-processor IBM SP, the Supercomputing Institute has recently acquired a 128-processor SGI Origin 2000 with 64 GB of memory. This machine has a processor speed of 195 MHz.

The Supercomputing Institute manages and operates both supercomputers and provides technical support to its users. The 256-processor IBM SP supercomputer and 128-processor SGI Origin 2000 are located at the Supercomputing Institute's facilities in the Minnesota Technology Corridor at the edge of the West Bank on the Minneapolis Campus of the University of Minnesota.

SGI/Cray Origin 2000 supercomputer housed at the Supercomputing Institute.

In addition to these supercomputers, the Supercomputing Institute has recently upgraded its IBM East Bank Laboratory, co-managed by the Supercomputing Institute and Computer Science Department, to include 72 processors with 36.5 GB of memory and 500 GB of disk. The Supercomputing Institute also offers its researchers access to a 32-processor SGI Origin 2000 with 8 GB of memory, an SGI Power Challenge, and a 2-processor Onyx2 as part of its Basic Sciences Computing Laboratory.

With these IBM and SGI resources and laboratories in the Supercomputer Center Building and Weaver-Densford Hall for scientific development, visualizations, and workstations, the Supercomputing Institute is providing its researchers with a diversified array of state-of-the-art tools.

To mark the arrival of the new 256-processor IBM SP supercomputer, the Supercomputing Institute hosted a dedication ceremony. The ceremony brought together faculty and student researchers of the Supercomputing Institute, representatives of the University's administration, representatives from IBM, and individuals whose efforts helped bring the supercomputer to the University.

The dedication ceremony featured remarks by Supercomputing Institute Director Professor Donald Truhlar, outgoing Vice President for Research Mark Brenner, incoming Vice President for Research Christine Maziar, Institute of Technology Dean H. Ted Davis, and Vice Provost for Graduate and Professional Education Norma Allewell. In addition, IBM Client Executive Patrick Carey presented the University of Minnesota with an IBM Shared University Research Award of IBM RS/6000 43P Model 240 workstations and a $25 million symbolic check that represented the money that IBM has given to the University of Minnesota in donations and grants over the years. Associate Vice President for Development and President of the University of Minnesota Foundation Gerald Fischer and Chair of the Board of Regents William Hogan were on hand to accept the award.

1998 Undergraduate Summer Interns

This summer, twenty-five undergraduate student researchers from the University and around the country served ten-week internship appointments at the Supercomputing Institute. The students were selected from a pool of over one hundred applicants to participate in programs in biophysical computing and computational dynamics as well as scientific computing and graphics. The students worked closely with faculty advisors on projects ranging from motion of a chain of rigid bodies to the modeling of a stent.

The Summer Internship Program is sponsored by the Supercomputing Institute and the National

Science Foundation's Research Experiences for Undergraduates Program, which is in its eighth year. The program promotes undergraduate involvement in ongoing and new research in many fields and provides students with an opportunity to work full-time on challenging and computationally intensive problems in an academic research environment.

During the course of the summer, the students participated in Institute sponsored tutorials specific to high-performance computing and in individual laboratory tours led by faculty members. To conclude the summer, the students presented talks open to the entire research community. These talks allowed them to share their work with other researchers and to gain experience making scientific presentations. The program allowed the students to perform research in close collaboration with faculty investigators and their research groups and to discuss research with faculty members, post-doctoral associates, graduate students, and other interns with similar interests.

Project Descriptions

Stefan Debbert, a Chemistry major at the University of Minnesota, worked with Professor Christopher Cramer of the Chemistry Department on computational chemistry approaches to understanding what influences effectiveness of antibodies on tumor cells. Since tumor cells are consistently more acidic than normal cells under certain physiological conditions, an antibiotic that is more reactive in the protonated form (one extra proton) than the unprotonated form may be able to preferentially attack tumor cells as opposed to healthy cells. Stefan looked at differences in pyridyne and benzyne electronic structures brought on by nitrogen's lone pair to observe effects and help determine the effectiveness of some of the antibiotics.

Derek Dolney worked with Professor Cramer and Professor Donald Truhlar of the Chemistry Department on calculating solvation free energies with the Conductor-Like Screening Model (COSMO), a method used to compute electrostatic portions of solvation free energies. Derek carried out the initial steps of developing the SM5CR solvation model (an implementation of the COSMO method) and incorporating it into the AMSOL software package. Performance of the model was evaluated by testing its accuracy for prediction of solvation free energies. The computation time required to complete such calculations with various choices of parameters was evaluated, and an optimum compromise of accuracy and cost was devised. Derek is majoring in Chemistry and Physics and minoring in Spanish at the University of Minnesota.

Mala Radhakrishnan is majoring in Chemistry and Physics and minoring in Philosophy at Harvard University. She worked with Professor Donald Truhlar of the Chemistry Department on calculating reaction rates. The first step toward a theoretical reaction rate calculation is optimizing geometries and determining electronic energies of the species involved. Mala first optimized the geometry of the reactants, products, and transition states of methanol, ethanol, and 2-propanol reactions using semi-empirical methods incorporated into the AMSOL computer package developed at the University of Minnesota. Using the methanol reaction as a prototype for more complex reactions, she analyzed accuracy, efficiency, and expense of other methods. A hybrid of the Hartree-Fock and density-functional theories was found to give sufficient flexibility to adjust calculated energies to agree with experiment. This combination was used to calculate the reaction rate of hydrogen with methanol in aqueous solution, and the results agree with experiment within experimental error. Nevertheless, future work is planned to explore the effect of nonequilibrium solvation on the tunneling contributions.

Jocelyn Rodgers, a Chemistry and Physics major at Harvard University, also worked with Professor Truhlar. Jocelyn calculated reaction rate constants for the reaction of hydroxyl (OH) radicals with alkenes and aromatic hydrocarbons. The OH radical is the single most important radical in combustion reactions. Jocelyn's project used the GAUSSIAN94 electronic structure package and the POLYRATE dynamics code for reaction of OH radicals with small unsaturated hydrocarbons. The applicability of this scheme for treating the reaction of OH with larger unsaturated organic compounds was a long-term goal. The electronic structure calculation involved as low an order of theory and as small of a basis set as possible to keep the expense of computing time down. This scheme can then be applied to larger hydrocarbons without being prohibitively expensive.

David Dreytser worked with Professor David Thomas of the Biochemistry Department on modifying the three-dimensional, atomic model of phospholamban, a fifty-two amino acid integral membrane protein of the sarcoplasmic reticulum. David wrote an algorithm to generate the relative orientation of helices in a bundle with desired geometries. This process required a reference helix chosen by finding the helical coordinate system of the first helix. Orientations of remaining helices were found by rotating every helix in the pentamer by identical angles. This process was repeated and the final structures were used to deduce a structure of phospholambam. David is majoring in Chemical Engineering and Biochemistry and minoring in Management at the University of Minnesota.

Ethan Bernard, a Biochemistry and Biophysics major at Oregon State University, worked with Professor David Levitt of the Physiology Department. A general method for simulating the motion of a chain of rigid bodies using a recursion relation had already been detailed. A recursion relation allows motion of an entire chain to be defined by motion of the first body and motion in the links connecting successive bodies. This method is different from a direct approach that simultaneously describes the chain with a system of equations and solves the equations to determine motion. Ethan wrote a program that simulated motion of the chain of rigid bodies using the direct method and tested this against a program using the recursion relation.

Seth Gammon, a Biophysics major at the University of Illinois at Urbana Champaign, also worked with Professor Levitt. Seth investigated characteristic change in chemical shift of a residue in a particular type of secondary structure. He used an automated approach to compare relationships between secondary structure and chemical shift. More specifically, beta turns, gamma turns, beta hairpin turns, alpha helixes, and beta sheets were looked at. Files containing Nuclear Magnetic Resonance (NMR) data were collected and narrowed down by specific criteria. If there was a choice between NMR ensembles or NMR averaged structures, the averaged structure was chosen. Seth wrote a C++ program to match up chemical shift data with appropriate structural information. Differences between standard chemical shift and reported chemical shift were determined and the data was statistically analyzed.

Eden Paster, a Biochemistry and Biology major at Rice University, worked with Professor William Gleason of the Laboratory Medicine and Pathology Department. Eden used a known three-dimensional structure of horse cytochrome *c*, determined by X-ray crystallography, to model for mouse cytochrome *c*. The amino acid sequences only differed by six amino acids, which allowed Eden to mutate the horse sequence into the mouse sequence. It was then possible to obtain a three-dimensional structure for mouse cytochrome *c* by submitting the amino acid

sequence to a modeling program. The structure was subjected to energy minimization and compared to structures obtained by different procedures. Eden then modeled the mouse cytochrome *c* interacting with mini-antibodies. A three-dimensional model of the antibodies was constructed, and quantitative data for a number of cytochrome *c* and miniantibody complexes was obtained.

Nhi Tran also worked with Professor Gleason. Nhi studied the three-dimensional expansion of a Palmaz-Schatz stent, a mechanical device used during balloon angioplasty (see www2.msi.umn.edu/Bulletin/Vol.14-No.3/july98.html). The system was modeled by finite element analysis methods as implemented in the commercial MARC/MENTAT package. Specific investigation dealt with the possibility of coating stents with biomaterials suitable for local drug delivery of therapeutic agents from the stent. Flexibility and resilience are required of stents to endure both deployment procedure and dynamic forces of cardiac contractions. These performance requirements translate into longitudinally flexible, corrosion-resistant, thromboresistant stents that need to be radially noncompliant, of high-expansion ratio, and in complete contact with the vessel wall. Nhi is majoring in Biomedical Engineering and minoring in Computer Science at Duke University.

Eric Hemmesch and **Timothy McMurry** worked with Professor Edward Egelman of the Cell Biology and Neuroanatomy Department on the installation and configuration of linux and supporting programs on a dual-processor computer. Their research began by looking at interactions between biological proteins and muscle fibers (actin and myosin). Electron micrographs allowed Eric and Timothy to visualize their conformations in a two-dimensional manner. Although these two-dimensional pictures offer great insight, they afford little information as to what occurs on the molecular level. Because of this, there is a need for a program to transform these images into three-dimensional structures that can be manipulated for a greater understanding of the atomic interactions. Eric and Timothy used Fourier-Bessel analysis in an attempt to recover three-dimensional information regarding the structure of the proteins. Eric is majoring in Chemical Engineering and Chemistry and minoring in Management at the University of Minnesota, and Timothy is majoring in Mathematics and Physics at Carleton College.

Gregory Wilde, a Biomedical Engineering major at Tulane University, worked with Professor David Thomas of the Biochemistry Department. Gregory helped determine the feasibility and applicability of molecular dynamics simulations for predicting electron paramagnetic resonance (EPR) spectra of spin-labeled myosin. In order to generate an accurate molecular dynamics trajectory, the project first found the most stable conformation and potential function of a spin-labeled myosin. This required a DISCOVERscript to minimize steric hindrance. A quick yet accurate model was decided upon. Once the structure was determined and recognized, a simulation was run to output orientation history of the spin label. If the system reached equilibrium, an order parameter was calculated to produce an EPR spectrum, and results were compared.

Michael Enz, a Physics and Computer Science major at the University of Minnesota, worked with Professor J. Woods Halley from the School of Physics and Astronomy on experiments involving low-temperature beams of atomic helium. Michael reproduced computer simulations of an experiment that applies current pulses to a resistive element covered by an adsorbed helium film creating a helium beam of evaporated atoms detected a few centimeters away by a superconducting bolometer. Michael's simulation assumed the evaporated atoms obey a classical,

Boltzmann distribution in velocity. Data with multiple peaks in the detected signal from high-power source pulses with thicker helium films were successfully described by a quantum evaporation theory based on unusual dispersion curves for quasi-particles in liquid helium.

Seth Van Oort, a Computer Science major at the University of Minnesota, worked with Professor David Lilja of the Electrical and Computer Engineering Department. Professor Lilja's group has been developing a program that takes data from a running program and displays it in an easily understood format. Seth worked on a segment of the project that would display data on the screen. A tree is the natural way to display methods. As the mouse is moved over each node, the data for that node is displayed. One of the major tasks involved in displaying the data was writing a function to search through a tree for nodes fitting certain parameters.

The source of some of the highest energy cosmic rays in our galaxy is still in question. The prevalent theory was that these high-energy particles are accelerated in the shock wave of a Supernova Remnant. **Johan Hoff**, majoring in Aerospace Engineering at the University of Minnesota, worked with Professor Thomas Jones of the Astronomy Department on a computer simulation of the progressive state of shock wave development and a numerical calculation of cosmic ray momentum distribution that could be generated by the modeled conditions. The simulation provided a calculable solution that accounted for observed and new theoretical results of high-energy cosmic ray studies. The simulation was performed on a hybrid, fluid-Boltzman-equation shock wave simulation code modified to take the effects of cosmic ray pressure and momentum in development of the shock wave into account.

Michael Greminger, a Mechanical Engineering major at the University of Minnesota, worked with Professor Charles C.S. Song of the Civil Engineering Department. Michael's project converted an existing FORTRANprogram into a parallel program that could run on a multiprocessor supercomputer or a network of workstations. He hoped conversion would increase speed allowing larger problems to be solved. Michael first tried automatic parallelization tools native to the supercomputers. He then tried parallelizing the program using Message Passing Interface, a library of functions that can be used to create parallel programs. Both methods were analyzed and compared.

Jeffrey Sommers worked with Professor Alon McCormick of the Chemical Engineering and Materials Science Department on three projects. The first dealt with the distance matrix, a mathematical entity that has proven useful in many fields. This work developed a program that used an efficient algorithm to compute the distance matrix for a given configuration of a certain number of atoms. The second project dealt with energies of various cyclic structures. The final project worked with diffusion simulations. Jeffrey began by writing a program that simulates diffusion in which the atoms can pass each other. The program was then modified so atoms could not pass each other. Jeffrey is majoring in Chemical Engineering and minoring in Chemistry at the University of Minnesota.

Steven Miller, a Chemical Engineering major at the University of Notre Dame, worked with Professor George Wilcox of the Pharmacology Department. Steven's project dealt with resolution of structures on sub-micron scales by confocal microscopy. This method is of value since a thick specimen may be optically sliced without damaging its structure, and images may be combined to render an object in three dimensions. The presence of out of focus light, noise, and other aberrations limit the usefulness of images for quantitative analysis. Mathematical deconvolution

restores the image to a better representation of the true object. An object of known morphology containing minute three-dimensional structures can test reliability of restoration and resolution of the microscope. A glass micropipette containing fluorescent dye was imaged at the tip where separation between compartments approaches the limit of resolution. By comparing restored images to structures established by electron micrograph, suitability of the method to quantitative analysis was determined.

Justin Sytsma also worked with Professor Wilcox. Justin is a Neuroscience and Computer Science major and Philosophy minor at the University of Minnesota. He simulated neurons using several mathematical models for comparison. One model was used for peripheral unmyelinated nerve fibers of the rabbit sciatic nerve. This model looked at a single point along the axon. Action potential was generated using a sodium current to produce initial depolarization. A leak current was used for repolarization. Once the best model was determined and code for the simulation was optimized, Justin used the model to look at effects on action potential propagation of the application of drugs to these fibers.

Rashid Zia worked with Professor David Yuen of the Geology and Geophysics Department and more than a half dozen researchers to transform portions of their models and simulations into a more communicative format. In the process, he became very familiar with several visualization programs. Aside from pure visualization, Rashid gained familiarity with both individual models and simulations of several researchers and the general styles of computer simulations. He has also become acquainted to general geothermal convection simulations, molecular dynamics simulations, and well-mixed data analysis models. Rashid is majoring in Electrical Engineering and American Literature at Brown University.

Andrew Shallue is majoring in Mathematics and minoring in Computer Science at Gustavus Adolphus College. He also worked with Professor Yuen. Andrew's project dealt with fractals and fractal theory. The most useful property of a fractal is its fractal dimension, which measures the ruggedness of a natural formation or graph. Andrew quantified the mixing process in mantle convection using fractal dimension and compared dimension over time with different mixing processes. Earlier work had analyzed mantle convection fields comparing differences in newtonian and non-newtonian rheologies over time. However, results were suspected to be inaccurate since fields are used more for visualization than analysis. With the development of the line method of modeling mantle convection, it became possible to more accurately quantify mantle mixing.

Christopher Messer, a Mathematics major at the University of Minnesota, worked with Professor Dennis Hejhal of the Mathematics Department. Professor Hejhal's research has illustrated chaotic phenomena in solutions to Schrödinger's equation for a quantum-mechanical particle of specific energy. Christopher studied the occurrence of this chaos within quantum-mechanical systems. He observed the solutions to Schrödinger's equation for a quantum-mechanical particle of specific energy that became increasingly chaotic as energy increased. Understanding the sources of this chaotic behavior led to a study on why such randomness can be present even in highly regular two-dimensional regions. Simplified cases with high symmetry in classical geometry were studied to aid identification of the factors that contributed to randomness.

Robert Roos, a Computer Science major at Stanford University, worked with Professor George Wilcox of the Pharmacology Department. Robert's project investigated feasible ways of counting

neurons. Many questions could be answered if a fast, reliable method of counting certain cells was available. In some cases, these questions involved the correlation between numbers of cerebellar Purkinje neurons and motor coordination of mice at varying ages and pathological states. While counting is in some ways the most basic type of data-gathering possible, it is extremely time-consuming. Robert's project aimed to automate the process, requiring that one of the central problems of computer vision-image recognition-be solved, to a high degree of accuracy, for the specific types of cells to be counted.

Heidi Basler is majoring in Computer Science and Mathematics and minoring in Physics at the University of Nebraska. She worked with Professor Leonard Banaszak of the Biochemistry Department in designing World Wide Web pages. Heidi learned to program in CHIMEsoftware, a plug-in that enables three-dimensional molecular structures of a protein to be placed on a World Wide Web page. Unlike other programs, CHIME displays live molecules that can be rotated and reformatted by users. CHIME allows text explaining proteins to be added with buttons to manipulate proteins and highlight regions, residues, and individual atoms.

Thomas Grys, a Biochemistry major at Gustavus Adolphus College, worked with Professor Douglas Ohlendorf of the Biochemistry Department on creating two sets of World Wide Web pages. One set provided descriptions of projects underway in Professor Ohlendorf's research group. These pages included active three-dimensional displays of macromolecules and links to other resources used by the group. This information is for candidates interested in studying at the University of Minnesota and the general public. The other set of pages was created for the 1999 International Conference for Biological Inorganic Chemistry being organized by faculty at the University of Minnesota. These pages allowed for online registration and submission of abstracts. A mechanism was set up to allow interested parties to search the archived abstracts for information about the projects and authors.

1998 Summer Tutorials, Laboratory Tours, and Intern Seminars

Introduction to the Supercomputing Institute
Introduction to Scientific Visualization
Introduction to Perl
Introduction to the IBM SP Supercomputer
Introduction to LoadLeveler and Batch Job Submission on the IBM SP Supercomputer
Math/Numerical Libraries for the IBM SP Supercomputer
Molecular Visualization Tools
Single Processor Tuning for the IBM SP Supercomputer
Data-Parallel Code Development on the IBM SP Supercomputer Introduction to InsightII/Discover
Introduction to Message Passing Interface
Point to Point Communication with Message Passing Interface
Collective Communications with Message Passing Interface
Advanced Message Passing Interface
Introduction to the SGI Origin 2000 Supercomputer
Math/Numerical Libraries on the SGI Origin 2000 Supercomputer
Data-Parallel Code Development on the SGI Origin 2000 Supercomputer
Introduction to Java Introduction to Shell Programming
Advanced Unix Features
Introduction to Parallel Programming

Astronomy laboratory tour
Biochemistry laboratory tour
Cell Biology and Neuroanatomy laboratory tour
Chemistry laboratory tour
Pharmacology laboratory tour
Physiology laboratory tour
Summer Intern Seminars

Future Program Information

The Supercomputing Institute is pleased to announce our summer 1999 internship program, open to both University of Minnesota and non-University of Minnesota undergraduate students. This program provides undergraduate students an opportunity for a challenging and enriching educational experience.

This internship is intended for undergraduate students interested in pursuing graduate or professional education and research in scientific computing and graphics. Students work with faculty on a wide variety of projects. Faculty from various disciplines have contributed projects and are responsible for directing the students in their daily work. Summer appointments will run from June 14 to August 20, 1999.

The Supercomputing Institute will also be providing Undergraduate Internships in Winter and Spring 1999. These internships will be available to University of Minnesota undergraduate students. Research projects will be available in a variety of disciplines. The winter program will run from January 4 through March 12, 1999. The spring program runs from March 29 to June 4, 1999.

Please check the Supercomputing Institute World Wide Web pages for more information.

Predicting Dissolved Contaminant Spread in Heterogeneous Ground Water Aquifers

Prediction of dissolved contaminant spread in ground water aquifers is necessary in designing ground water protection and remediation measures. These predictions are usually accomplished by solving the convection-dispersion equation (CDE). The dispersion coefficient in the CDE is assumed to be constant in standard practice, but this coefficient is now recognized to depend on space and time.

The research team of Professor John L. Nieber, Graduate Students AbdelKarim Abulaban, Paul Oduro, and Hung Nguyen, and Research Associate Cam Nguyen of the Biosystems and Agricultural Engineering Department at the University of Minnesota have undertaken an effort to quantify effects of multiscale spatial heterogeneity on solute plume spread. In addition, they are working on ways to estimate the dispersion coefficient in natural porous media. In this work, solute plumes are simulated using a particle tracking random walk solution of the CDE. This work is being accomplished in cooperation with Dr. John Peters and Dr. Stacy Howington from the United States Army Waterways Experiment Station Laboratory in Vicksburg, Mississippi. This cooperation is supported by the Army High-Performance Computing Research Center at the

University of Minnesota.

Sample results of the current work are shown in Figures 1 and 2. Sample ground water velocity fields are shown in four different conditions for an aquifer with dimensions of 200 meters by 2000 meters. In Figures 1a-1c, velocity fields for various levels of hydraulic conductivity (K_2) heterogeneity are shown. For each field, the hydraulic conductivity is statistically homogeneous (constant mean and variance of K_2). Note that the color scale for each graph is relative to the maximum value of the variable depicted in that graph. The variable σ represents the standard deviation of ln(K_2) and L represents the spatial correlation of ln(K_2). In contrast, the velocity field shown in Figure 1d is for the condition where multiple scales of K_2heterogeneity (mean and variance of $K_2$are not constant) are represented. Solute plumes for a conservative solute (non-sorbing, non-degrading) were generated using each of these velocity fields, and the plume at 500 days associated with each velocity field is displayed immediately beneath the associated velocity field plot. It is observed in Figures 1a-1c that the solute plume spread increases as the values of σ and L increase. The plume in Figure 1d is even more spread, showing the effects of the multiple scales of heterogeneity. The simulation of the solute plume for each velocity field was performed using 200,000 particles with the solute initially concentrated within a 10 m^2 area. Each of these simulations required a high- resolution representation of the aquifer hydraulic conductivity.

Further research is attempting to mimic high-resolution simulations with a simpler particle tracking model. The simpler model incorporates multiscale spatial heterogeneity into a random velocity generator superimposed onto a mean flow field. Because of this, high-resolution representations are not needed. A solute plume generated with this approach is shown in Figure 2.

In future research, this group will derive parameters from the high-resolution fields to be input into the simpler dispersion model. This work will make it capable to closely predict behavior of the high-resolution simulations. Further work will investigate the effects of solute sorption, multicomponent chemical reactions, and biodegradation on solute plume behavior when multiscale spatial heterogeneity is present.

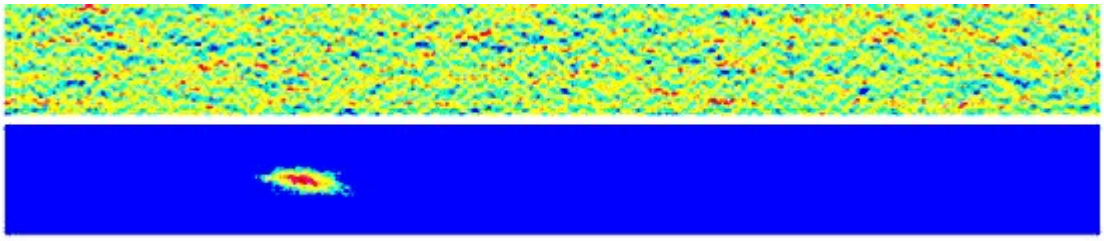


Figure 1a:

Longitudinal velocity and concentration profile of ground water for σ = 0.5 and L = 5 m.

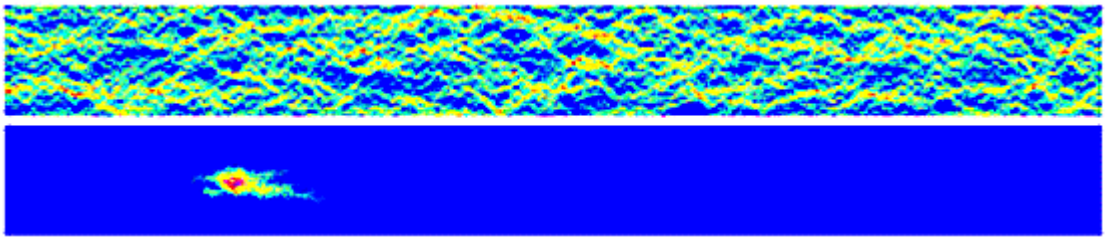


Figure 1b:

Longitudinal velocity and concentration profile of ground water for σ = 1.0 and L = 10 m.

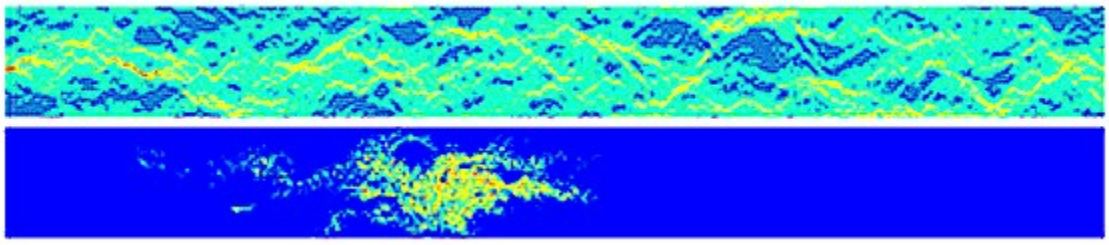


Figure 1c:

Longitudinal velocity and concentration profile of ground water for $\sigma = 2.0$ and $L = 20$ m.

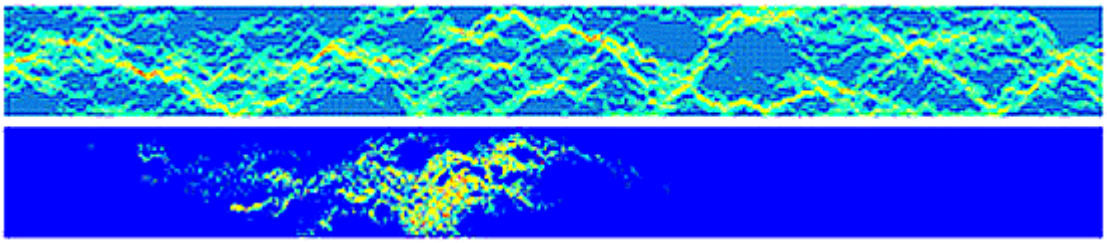


Figure 1d:

Longitudinal velocity and concentration profile of ground water for the sum of the hydraulic conductivity fields for figures 1a-1c.

Figure 2: A solute plume generated with a random velocity generator, representing multiscale spatial heterogeneity, superimposed onto a mean flow field.

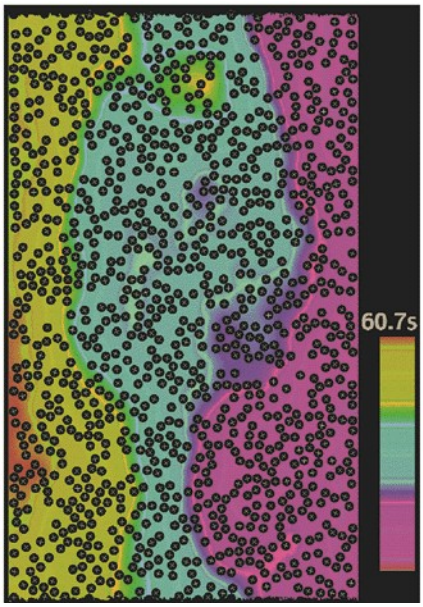
Direct Numerical Simulation of Liquid-Solid Flow

This project is sponsored by a National Science Foundation Grand Challenge high-performance computing grant and by several industrial partners (Dowell- Schlumberger, Schlumberger, Shell, Stimlab, and Intevep, S.A.). In this project, particles are moved by Newton's laws under the action of hydrodynamic forces computed from the numerical solution of the fluid equations. Solutions of the initial value problem for dispersions of solid particles in fluidized beds, slurries, sand placement in fracture oil reservoirs, cleaning of drill cuttings from oil wells, and other applications are solved without approximations beyond those inherent in simulations.

A goal of the project is to develop state-of-the-art software packages for solving initial-value problems for dispersions of thousands of particles on parallel computers. To achieve this, a marriage between computational fluid dynamics (CFD) and computer science (CS) is created to produce the most efficient parallel preconditioners and iterative schemes. These are needed to handle the large nonlinear and linear algebraic equations that arise in this investigation. These solutions consume the largest percentage of the simulation time.

Regents' Professor Daniel Joseph of the Aerospace Engineering and Mechanics Department at the University of Minnesota is the principal investigator, Roland Glowinski of the Mathematics Department at the University of Houston and Howard Hu of the Mechanical Engineering and Applied Mechanics Department at the University of Pennsylvania are co-principal investigators on the CFD side, and Yousef Saad of the Computer Science and

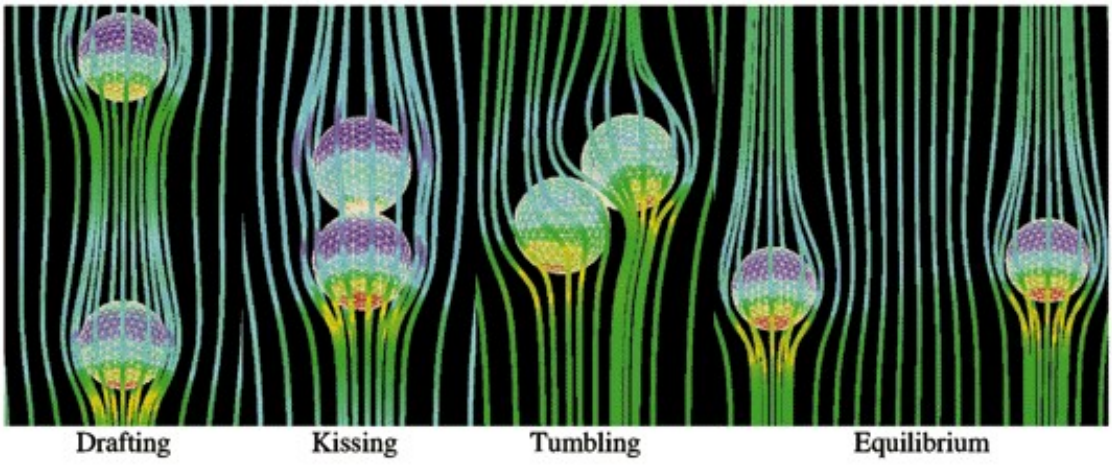
Engineering Department at the University of Minnesota and Ahmed Sameh of the Department of Computer Sciences at Purdue University are the co-principal investigators on the CS side.



1,109 particles flowing in a Newtonian fluid in a channel. The mixture is pumped upwards against gravity. Color shows the stream function.

The collaboration of these two communities, which traditionally speak different languages, has given rise to an interdisciplinary group that communicates with ease across disciplinary boundaries. This interdisciplinary research effort has already resulted in two state-of-the-art parallel software packages. The first, which uses a moving unstructured body fitted grid, is the only numerical package anywhere that can move solid particles in a viscoelastic fluid in direct simulation. The second is an elegant package that uses a fixed grid in which particles are represented by a field of Lagrange multipliers associated with the constraint of rigid body motion. The fixed structured grid offers opportunities for using rapid solvers that are ideally suited for parallel implementation. Performance results obtained on two parallel computational platforms, an SGI Origin 2000 and a Cray T3E, indicate that routine fine tuning of various kernels results in efficient utilization of the parallelism offered by these architectures. A further aim is to produce industrial-strength counterparts of the codes that are portable across a variety of parallel architectures.

Both software packages use a new, combined weak formulation. In this formulation, the fluid and particle equations of motion are combined into a single, weak equation of motion from which hydrodynamic forces and torques on the particles have been eliminated. These and other results achieved in this Grand Challenge project have opened new and promising lines for investigation. Further details are available at: www.aem.umn.edu/Solid-Liquid_Flows.



Interactions between two spheres sedimenting in a tube. The lines are streamlines, and color indicates the pressure field.

Short Contact-Time Reactors: Two-Dimensional Modeling Including Detailed Chemistry Models

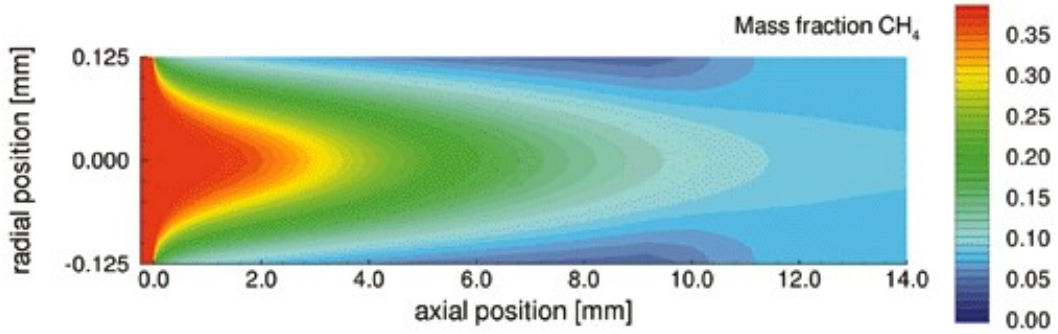
Reaction engineering and combustion processes are often characterized by a complex interaction of transport and chemical kinetics. The chemistry may include gas-phase as well as surface reactions. Direct partial oxidation of light alkanes, the main components of natural gas, in short contact time reactors have been shown to offer a promising route to convert light alkanes into more useful chemicals such as syngas (H_2 and CO), olefins, and oxygenates. Catalysts used for these processes include foam or extruded monoliths, wire gauzes, or sintered spheres that are coated with noble metals such as platinum and rhodium. The reactor can be

run autothermally and almost adiabatically with a residence time of approximately one millisecond. Short contact time guarantees a very high throughput using a small amount of catalyst and low energy and capital costs. However, the industrial application needs to operate at higher pressure, but high-pressure experiments in conventional laboratories are expensive and dangerous because reactive mixtures may explode. Detailed modeling and simulation help to clarify complex interactions between reactive flow and catalytic surfaces and can be used to explore reactor conditions beyond available experimental facilities.

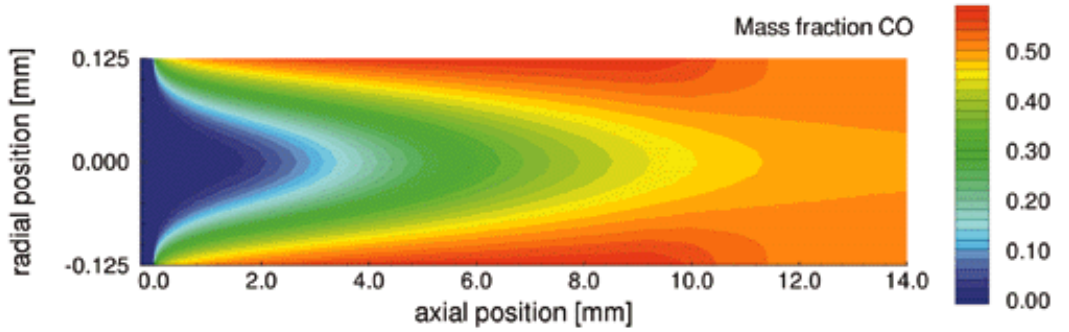
This work is being carried out by Professor Lanny D. Schmidt and Dimitrios Iordanoglou, a Graduate Student Researcher, of the Chemical Engineering and Materials Science Department at the University of Minnesota and Olaf Deutschmann, a Research Associate, now at Heidelberg University in Heidelberg, Germany. They developed a computer program to simulate short contact time reactors using a two-dimensional flow field description and detailed models for surface and gas-phase chemistry. The program was based on the commercial computational fluid dynamics (CFD) code fluent. The current version of this code, although able to handle multi-species flow including diffusion and heat transfer, is not capable of simulating flows that include a large number of stiff chemical reactions. Therefore, fluent was coupled with models created by the group that simulate gas phase as well as surface chemistry.

The extended CFD code was then used to model the partial oxidation of methane on Rh and Pt in a short contact time reactor containing a catalytic foam monolith. The simulation included 22 surface reactions and 164 gas phase reactions. Reaction pathways, interaction between convection, diffusion, adsorption/desorption processes, and surface chemistry were elucidated. The importance of gas phase chemistry at higher pressures were revealed. The figures show how the reactant methane is consumed and CO, one of the desired products, is formed. Furthermore, the formation of OH radicals are shown. These OH radicals act as a precursor to the undesired combustion products carbon dioxide and water. Recently, these researchers also used this computer program to simulate partial oxidation of methane over platinum gauzes.

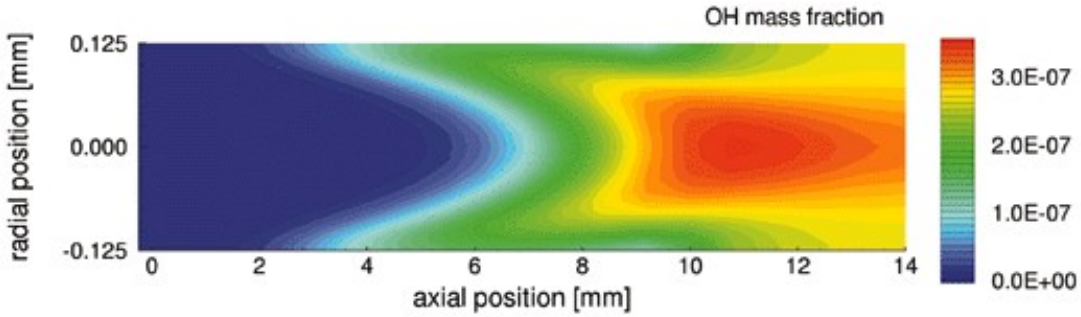
In the future, this group will improve surface reaction mechanisms of hydrocarbon oxidation over noble metals. Group members will also incorporate detailed gas-phase chemistry for larger hydrocarbons in their calculations. These studies are very crucial for a detailed understanding of short-contact-time reactors. This knowledge is necessary for an efficient scale-up of laboratory-scale reactors to commercial applications.



Mass fraction of methane in the reactor channel.



Mass fraction of carbon monoxide in the reactor channel.

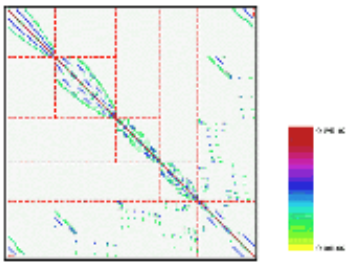


Mass fraction of OH radicals in the reactor channel.

future symposium

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

June 10–12, 1999



The innermost computational kernel of many large industrial numerical simulations is a large sparse matrix linear system. A recent survey indicated that more than 70% of supercomputer time is used for solving large linear systems. A great impact can be made if performance of these sparse matrix solvers can be improved.

Storage requirements for three-dimensional simulations make direct methods prohibitively expensive. Iterative techniques become mandatory but lack the robustness of direct methods. Past emphasis has been devoted to exploring more powerful iterative solvers. These techniques did not have much initial impact, and experience indicates that a good preconditioner holds the key to an effective iterative solver.

This conference, sponsored by the University of Minnesota Supercomputing Institute and the University of Waterloo in cooperation with SIAM Linear Algebra Group, brings researchers and engineers together to discuss recent developments and progress made as well as to exchange findings and explore possible new directions in this field.

Invited speakers include Raymond Chan from The Chinese University of Hong Kong, Edmond Chow from Lawrence Livermore National Laboratory, Howard Elman from the University of Maryland, Charbel Farhat from the University of Colorado, Peter Forsyth from the University of Waterloo in Canada, David Keyes from the NASA Langley Research Center, John Lewis and Dan Pierce from Boeing Computer Service, Maya Neytcheva from the University of Nijimegen in The Netherlands, Willy Schilders from Philips Research Laboratories, Henk van der Vorst from Utrecht University in the

Netherlands, and Justin Wan from Stanford University. Contributed papers are being solicited.

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Registration and Contributed Papers

Information about registration and contributing papers is available by sending email to sparse99@msi.umn.edu or at: www2.msi.umn.edu/Symposia/sparse99

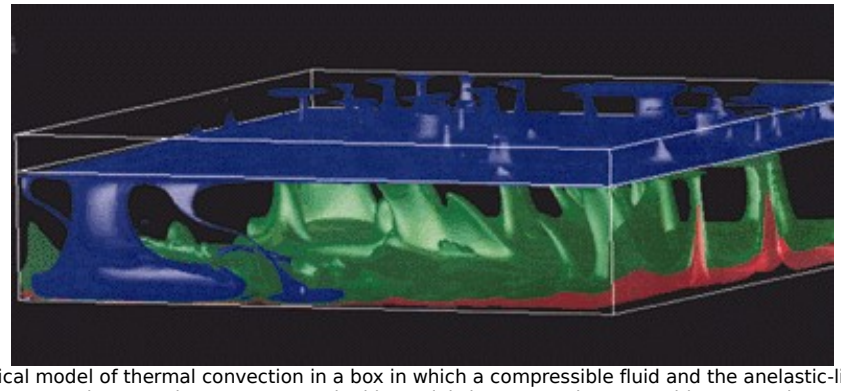
visitors

British Broadcasting Company

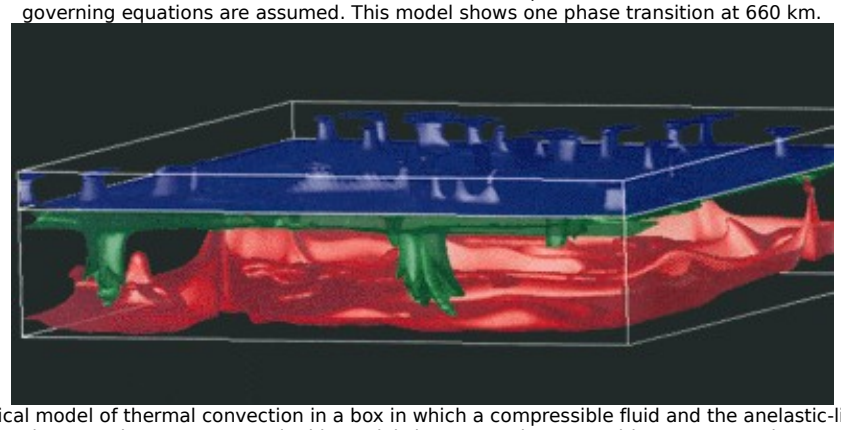
David Hutt of the British Broadcasting Company and his crew recently came to the Supercomputing Institute to interview Professor David Yuen of the Geology and Geophysics Department of the University of Minnesota and Fellow of the Supercomputing Institute on the topic of mantle plumes and massive basaltic magma outpouring resulting from plumes impinging on the oceanic plate under the Pacific Ocean and the continental region under Siberia 225 million years ago. Recent geophysical evidence shows layering in the lower part of the mantle transition zone down to a depth of 1,000 km. Seismic observations have revealed a reflector surface at around 900 or 1,000 km depth for which a possible explanation can be given in terms of a new phase transition of the lower-mantle constituent minerals. Furthermore, new attempts on the inversion of the oceanic geoid show the existence of a second low viscosity zone somewhere between 660 and 1,000 km depth. The existence of the second low viscosity zone may be linked to the mid-mantle phase transitions.

High-resolution, three-dimensional numerical simulations by Dr. Laszlo Cserepes, a collaborator in Professor Yuen's research group, from the Eotvos University in Budapest, Hungary were visualized by undergraduate research assistants from Professor Yuen's group, Josh Collins and Brigit Schroeder. These simulations (see figures) include phase and viscosity stratification of the transition zone in three dimensions in a 4 x 4 x 1 rectangular box. A hypothetical weak endothermic transition at 1,000 km was assumed in some of the models. When the 1,000 km endothermic phase transition is included, these instabilities can grow only at a few places, but they form strong downwellings. Two distinct types of penetrative, deep downwellings can be present at the same time: one that crosses the whole transition zone, and another that crosses only the 660 km discontinuity and stops at 1,000 km (at least temporarily). This can explain seismological observations that suggest that subducted slabs can be retarded not only by the 660 km boundary, but also by some deeper obstacle near 1,000 km depth.

These visualizations were filmed by David Hutt's crew for display. The hour long special has already been shown in England and is now being distributed to television networks around the world.



Three-dimensional numerical model of thermal convection in a box in which a compressible fluid and the anelastic-liquid approximation of the governing equations are assumed. This model shows one phase transition at 660 km.



Three-dimensional numerical model of thermal convection in a box in which a compressible fluid and the anelastic-liquid approximation of the governing equations are assumed. This model shows two phase transitions at 660 and 1,000 km.

visitors

Nara Institute of Science and Technology

The Biological Process Technology Institute (BPTI) at the University of Minnesota recently began an exchange program with the Nara Institute of Science and Technology (NAIST). This agreement provides an exchange of academic personnel, information, and materials and is now working to organize a joint sumposia and initiate research between the University of Minnesota and NAIST. The typical exchange encompasses a three week period. Dr. Doug Hershberger of BPTI hosted five members of NAIST over the summer.

The purpose of these collaborations is twofold. First, research is being planned in the areas of informatics, plant biotechnology, and bioremediation. Second, the two schools have begun work on a joint international symposium on biocatalytic processing and bioremediation to be held in Nara, Japan. The two groups will exchange personnel soon to begin working out details of this symposium.