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Computational Biology for the Spectral Tuning of Visual Pigments

The ability for the human eye to distinguish a variety of shades of color is entirely determined by the chromo-phore 11-*cis* retinal, which is covalently connected through a protonated Schiff base likage to a lysine residue at position 296 of the transmembrane-protein rhodopsin. Human visual pigments are found in the rod and cone cells that line the outer layer of the retina. The rod cells contain pigments, that are responsible for dark vision with a maximum absorption wavelength (l_{max}) at 500 nm. The cone cells, which contain three pigments with l_{max} preferentially at 425 nm (blue), 530 nm (green), and 560 nm (red), are responsible for color vision. The spectral properties are characterized by the opsin shift, which refers to the difference between the observed l_{max} of the retinal protonated Schiff base in methanol solution and that in the protein environment (see Figure 1). Note that the protonated Schiff base has a different conformation in solution in the 6-*s*-*cis* form from the bacteriorhodopsin, where it is 6-*s*-*trans*.

A major goal in vision research is to elucidate the origin of the opsin shifts and the molecular mechanism of color regulation. Supercomputing Institute Fellow Jiali Gao, Professor of Chemistry and Digital Technology Center faculty, with his research group is developing methods that combine quantum and molecular mechanics (QM/MM) to model the force field for molecular dynamics simulations of biological processes. These methods can be applied to enzymatic reactions and photochemical processes in proteins. The basic idea of combined QM/MM methods is to partition a large molecular system into a small, primary region, which is treated quantum mechanically and also a region consisting of the remaining protein-solvent system. The much larger protein-solvent system is represented by molecular mechanics force fields that are less computationally demanding than the

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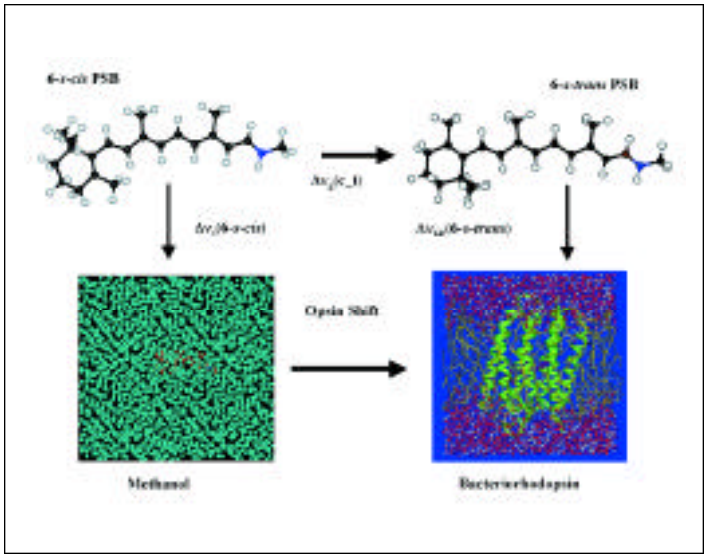

Figure 1. Energetic cycle used to define the opsin shift. The top arrow corresponds to isomerization in the gas phase, and the two vertical arrows correspond to inserting the protonated Shiff base into liquid methanol or into the protein. In all cases $\Delta\upsilon$ denotes the shift in spectral frequency.

Also in this issue

quantum mechanical calculations. Their approach for studying the opsin shifts is based on a procedure developed recently for simulation of membrane proteins and for the calculation of solvatochromic shifts of organic chromophores in solution. The method relies on an electronic structural technique called the configuration interaction (CI) method for the treatment of the protonated Schiff base, which is embedded in rhodopsin and lipid membrane. By including single excitations in configuration interaction calculations (CIS) using modest basis sets (6-31G(d) and 3-21G), Professor Gao and graduate student Ramkumar Rajamani first modeled the transmembrane protein bacteriorhodopsin and then extended their studies to probe specific contributions of individual amino acids to the spectral tuning in the visual pigment rhodopsin.

To relate the experimental opsin shifts to computational models, the researchers carried out statistical mechanical Monte Carlo and molecular dynamics simulations of the protonated Schiff base in methanol solution and in the trans-membrane proteins, bacteriorhodopsin and rhodopsin, using the combined QM-CIS/MM method described above.

Professor Gao and Rajamani obtained a theoretical opsin shift of 5200 cm^{-1} in bacteriorhod-opsin, which is in excellent agreement with the experimental value of 5100 cm^{-1}. The researchers analyzed the contributing factors to the opsin shift and found that both solvation and interactions with bacteriorhodopsin significantly shift the absorption maximum of the protonated Schiff base, but the effects are much more pronounced in a polar solvent such as methanol than in the protein environment. The differential solvatochromic shifts in methanol and in bR leads to a bathochromic (red) shift of about 1800 cm^{-1}. The extension of the p-conjugated system further increases the red shift by 2400 cm^{-1}. The remaining factors are due to the change in dispersion interactions, which have an estimated value of about 1000 cm^{-1}.

Using the same simulation approach, Rajamani also studied the opsin shifts in the visual pigment rhodopsin. The best computational estimate of the opsin shift is 2100 cm^{-1}, which is in approximate accord with experiment (2730 cm^{-1}).

An important question is how individual amino acid residues interact and regulate the absorption energy of the protonated Schiff base in the visual pigments. They examined the effects of four amino acid mutations that produce opposite spectral effects. Figure 2 shows residues in close contact with the protonated Schiff base in rhodopsin. Overall, the observed trends of spectral shifts due to mutations are reproduced in the present combined QM/MM study.

The study by Professor Gao's group on the spectral shifts in transmembrane proteins is especially exciting because it suggests that accurate molecular dynamics simulations of the photoisomerization processes can be studied using combined QM/MM methods.

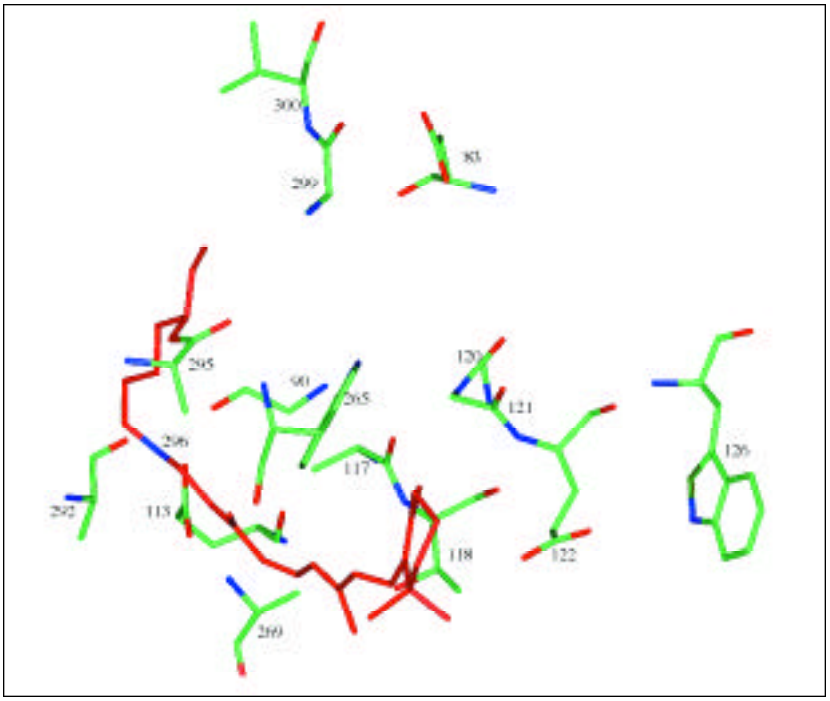

Figure 2. Residues in contact with the protonated Shiff base.

Simulations of Turbulent Transport in the Atmospheric Boundary Layer

Hydrologic, weather, and climate models require the estimation of turbulent fluxes of heat, momentum, and water vapor near the land surface. Measurement and modeling of these fluxes at regional scales (~10-100 km) is challenging due to the complex multiscale interactions between land surface heterogeneity and turbulence in the atmospheric boundary layer (the lowest part of the atmosphere). The goal of Professor Fernando Porté-Agel, Civil Engineering, and his research group is to better understand and model land-atmosphere exchanges through a combination of theoretical, experimental (field and wind tunnel studies) and numerical techniques.

Recently, the use of computational fluid dynamics, in particular large-eddy simulations (LES), has become a promising tool to study the complex dynamics of land-atmosphere interactions. LES consists of solving the three-dimensional unsteady transport equations for momentum and scalar variables such as temperature and water vapor in turbulent flows. Porté-Agel's research group has developed an LES code to study turbulent transport in the atmospheric boundary layer. They perform simulations of the atmospheric flow in spatial domains of about 10 km in the horizontal directions and 1 km in the vertical direction, with a grid resolution of approximately 10m. Figure 1 shows the simulated, instantaneous, three-dimensional temperature field corresponding to a boundary layer over a heterogeneous land surface (characterized by remote sensing) during a summer day. Note how the simulation captures the dynamics of buoyant plumes developing over warm spots, rising up, and mixing into the relatively cooler boundary layer.

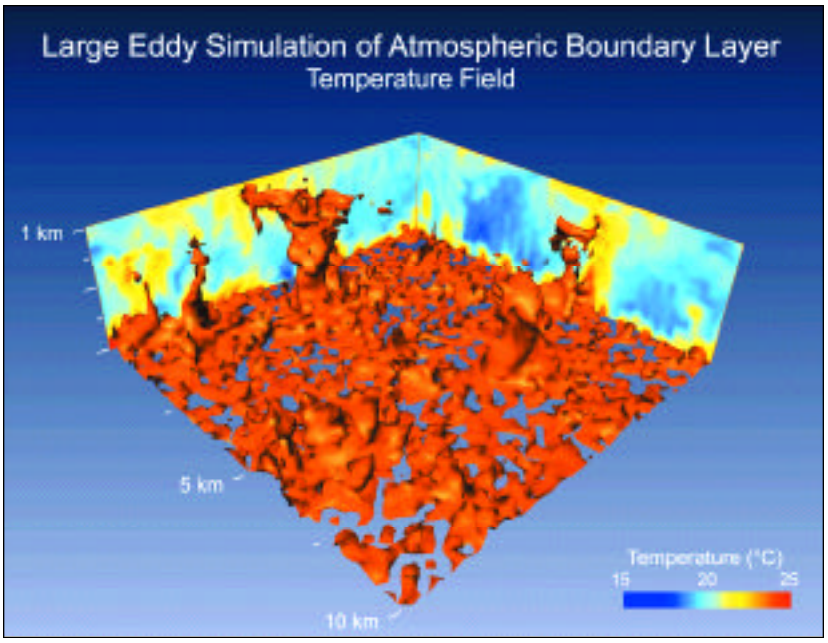

Figure 1. Instantaneous temperature field obtained from a large-eddy simulation of the atmospheric boundary layer over a heterogeneous surface.

Professor Porté-Agel and researchers Robert Stoll, Matthew Carper, and Nenad Bjelogrlic use simulation results to achieve the following objectives: 1) development of improved, physically realistic subgrid-scale models required to account for the effect of non-resolved, smaller than the grid size physics in models of environmental and engineering turbulent flows; 2) development of web-based visualizations/animations of atmospheric boundary layer turbulence for educational purposes (see: LES.safl.org); 3) quantification of the impact of land surface heterogeneity on the dynamics of the boundary layer and on the magnitude of the regional-scale fluxes. These results are leading to improved parameterizations of non-linear land-atmosphere exchanges and, consequently, increased accuracy of hydrologic, weather, and climate models.

Improving the Efficiency of Sparse Matrix Storage

A large number, if not the majority, of the computational problems encountered in scientific computing lead to matrix equations involving large sparse matrices. A matrix is said to be *sparse* if most of its entries are nonzero. Efficient techniques exist which avoid or reduce the storage of zero elements. These work only with the nonzero entries, while attempting to introduce as few new nonzero entries (fill-ins) as possible.

Researchers face the difficulty of selecting a suitable method or even a simple, general approach for handling sparse matrices. Should one use MATLAB? What tools and methods are available in the public domain to solve these problems? How does one store a sparse matrix? Is a direct method preferable to an iterative method? A Fortran library called SPARSKIT* was developed in the early 1990s to help handle sparse matrices. SPARSKIT includes subroutines that range from very simple functions (for example, adding two sparse matrices or extracting a given diagonal from a sparse matrix) to more complex suites of iterative solvers. Other packages exist which are mostly oriented toward providing solvers.

During the past five years, MATLAB** has developed support for sparse matrices; however, not all functions available for dense problems are available for sparse problems, therefore support is limited. Similarly SCILAB, a public domain package similar to MATLAB that was developed by the Institut National de Recherche en Informatique et en Automatique (INRIA) in France, incorporates options for working with sparse matrices. A group in Rennes, France, has recently coupled SPARSKIT with SCILAB.

Over the last few years, Supercomputing Institute Fellow Yousef Saad, Department of Computer Science and Engineering, and three Supercomputing Institute undergraduate interns developed an interactive interface to SPARSKIT, called SparseMath or SPMATH (Figure 2). Peter Braten, a 1994 and 1995 Supercomputing Institute summer undergraduate intern, developed the first C++ classes and initial grammar used to obtain the command interpreter of SPMATH. SPMATH uses LEX and YACC, two standard tools for parsing and interpreting commands. Marie Sauvaud, a telecommunications engineering student from Brittany, France continued Braten's work in 1999 by adding functionality to the package. Marie developed an option to load written programs, similar to the .m files in MATLAB. She also added an interface to all the solvers in SPARSKIT. Benjamin Langmead, Columbia University Computer Science undergraduate and 2001 Supercomputing Institute intern developed a Total Command Language/Toolkit (TCL/TK) graphics interface.

These developments have resulted in an interactive tool with improved functionality. Researchers can use it to conduct a quick test (e.g., trying an iterative method on a given problem) or for visualizing the sparsity pattern of a matrix. In addition, options for colors, zooming, and interactive information on the matrix are available. SPMATH provides user access from an intuitive command-line environment to a large set of sparse matrix functions provided through SPARSKIT, thereby assisting with complicated development work on iterative methods. SPMATH's syntax is

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* Y. Saad, "SPARSKIT: A basic tool kit for sparse matrix computations," *Technical Report RIACS-90-20*, Research Institute for Advanced Computer Science, NASA Ames Research Center, Moffet Field, CA, 1990.
see www.cs.umn.edu/~saad/software.html

** MATLAB is a trademark of MathWorks, Inc.

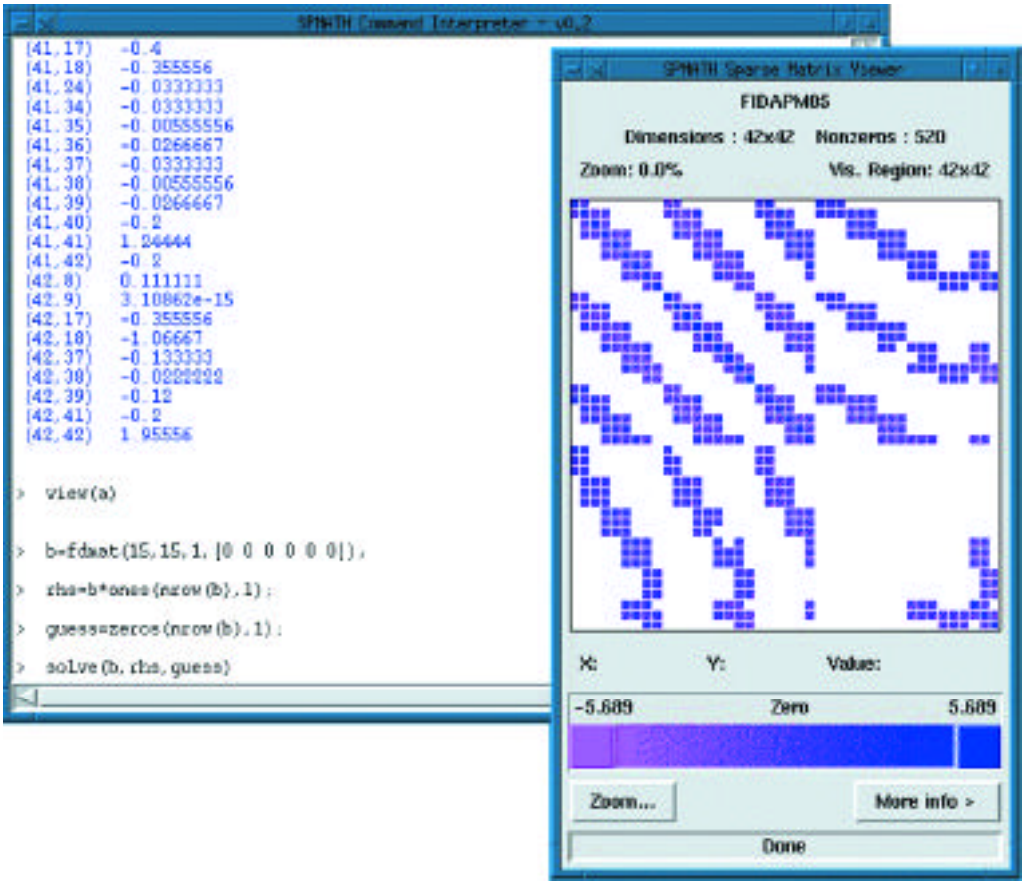

Figure 1. SparseMath (SPMATH) is an interactive tool based on the SPARSKIT library, which allows the user access to a powerful set of sparse matrix functions from an intuitive command-line environment. In addition to the command-line environment, SPMATH includes a toolkit-based visual interface. A sparse matrix viewer is included for quick visualization of results.

similar to MATLAB and SCILAB basic matrix operations.

Currently, the development goal is to continue adding functionality to the package. In particular, a number of ancillary functions such as standard plotting routines are needed. Adding functionality and improving the package "one brick at a time" has proven to be an effective strategy.

If you wish to use this free SPMATH software program, please download it from: http://www.cs.umn.edu/~saad/spmath.

34th Annual Midwest Theoretical Chemistry Conference

The 34th Annual Midwest Theoretical Chemistry Conference (October 5-6, 2001) brought together researchers and students in the areas of theoretical chemistry. The conference was designed as a platform for senior scientists (faculty and other senior researchers) to present their research and accomplishments in plenary sessions and for students and postdoctoral associates to give poster papers.

The conference was organized by the Minnesota Computational Chemistry Group (MC^2) consisting of University of Minnesota faculty, Christopher J. Cramer, Jiali Gao, J. Ilja Siepmann, Donald G. Truhlar, and Darrin M. York, and sponsored by the Supercomputing Institute, the Army High Performance Computing Research Center, IBM, SGI, Compaq, and Cray, Inc. The plenary speakers (in alphabetical order) and the titles of their talks are listed on the next page.

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Top: Katherine Hunt, Michigan State University, Karl Freed, University of Chicago, and Larry Curtiss, Argonne National Laboratory, MTCC Plenary Speakers.

Center: Nathan Knotts and John Adams review poster papers during one of two poster sessions.

Bottom: Jerry Leszczynski, Jackson State University, MTCC Plenary Speaker.

Conference speakers:

- Daniel M. Chipman, University of Notre Dame, *Reaction Field Theory for Electronic Structure*
- Christopher J. Cramer, University of Minnesota, *New Developments and Applications of SMx Models*
- Larry A. Curtiss, Argonne National Laboratory, *Computational Thermochemistry Using Gaussian-3 Theory*
- Ernest Davidson, Indiana University, *A Computational Verification of the Relation of Dyson Orbitals to Kohn-Sham Orbitals*
- Michael Davis, Argonne National Laboratory, *Geometric Approach to Multiple-Time-Scale Kinetics*
- Jerry R. Dias, University of Missouri at Kansas City, *Unified Structure Theory of Benzenoid Hydrocarbons*
- Clifford Dykstra, Indiana-Purdue University at Indianapolis, *Slipperiness on Sticky Intermolecular Interaction Surfaces*
- Karl Freed, Universityy of Chicago, *IVO-CASCI Method as a Replacement for CASSCF Calculations in Electronic Structure Packages*
- Jiali Gao, University of Minnesota, *Combined QM/MM Simulations of Enzymatic Reactions and Membrane Proteins*
- J. Daniel Gezelter, University of Notre Dame, *A Reductionist Model for Biological Membranes*
- Rainer Glaser, University of Missouri at Columbia, *Theoretical Studies of DNA Base Deamination*
- Mark Gordon, Iowa State University, *Chemistry at the Silicon (100) Surface*
- Stephen Gray, Argonne National Laboratory, *Real Wave Packet Approach to the Quantum Dynamics of Four-Atom Systems*
- Christopher M. Hadad, The Ohio State University, *Conformational Analysis of Carbohydrates Containing Arabinofuranosyl Rings*
- Lawrence B. Harding, Argonne National Laboratory, *Radical-Radical Recombination Reactions*
- William Hase, Wayne State Univ., *Dynamics of Central Barrier Crossings in Gas Phase $X^- + CH_3Y$ S_N2 Nucleophilic Substitution Reactions*
- Katharine Hunt, Michigan State University, *Nonlocal, Intramolecular Dielectric Functions*
- Jan Jensen, University of Iowa, *The EFP Method: Theory and Biochemical Applications*
- Steven R. Kass, University of Minnesota, *Probing Electrostatic Effects via Experiment and Theory*
- Samuel Krimm, University of Michigan, *Spectroscopically Determined Polarizable Force Fields for Macromolecules*
- Jerzy Leszczynski, Jackson State University, *Molecular Structures and Properties of Complexes with Weakly Interacting Ligands: Shells and Shellvents*
- Nancy Makri, University of Illinois at Urbana Champaign, *Quantum Dynamics of Large Systems: Recent Developments and Applications*
- Todd Martinez, University of Illinois at Urbana-Champaign, *Generalized Electronegativity and New Models for Charge Transfer*
- Glenn Martyna, Indiana University, *Folding Atomistic Models of Proteins on Computers*
- Anne McCoy, The Ohio State University, *Diffusion Monte Carlo Studies of the Structure and Spectra of Weakly Bound Complexes*
- Piotr Piecuch, Michigan State University, *New Coupled-Cluster Methods for Molecular Potential Energy Surfaces and Excited States*
- Mark Ratner, Northwestern University, *Some Notions About Molecular Junctions, and Transport in Them*
- Stuart A. Rice, University of Chicago, *Quasi-Two-Dimensional Systems: Structure and Dynamics*
- Stuart Rothstein, Brock University, *Quantum Monte Carlo Study of Static Electrical Properties of Atoms and Molecules*
- George Schatz, Northwestern University, *Metal Nanoparticles and Nanoparticle Aggregates*
- H. Bernhard Schlegel, Wayne State University, *Exploring Potential Energy Surfaces for Chemical Reactions Using Electronic Structure Methods*
- David M. Schrader, Marquette University, *Antimatter Systems via Quantum Monte Carlo*
- J. Ilja Siepmann, University of Minnesota, *Simulating Microheterogeneous Fluids*
- James Skinner, University of Wisconsin at Madison, *Spectroscopy and Dynamics in Liquids*
- Xueyu Song, Iowa State University, *The Role of Anisotropic Interaction in Protein Crystallization*
- Jason Thompson, University of Minnesota, *Dirac Award Lecture, Reactions of Hydroxide with Chlorinated Hydrocarbons*
- Donald G. Truhlar, University of Minnesota, *Chemical Dynamics Research*
- Olaf Wiest, University of Notre Dame, *Pericyclic Reactions of Radical Cations*
- Angela Wilson, University of North Texas, *Extensions of Ab Initio Methodology to Chemical Systems of Intermediate and Large Size*
- Arun Yethiraj, University of Wisconsin at Madison, *Dynamics of Polyelectrolyte Solutions*
- Darrin M. York, University of Minnesota, *Multi-scale Quantum Models to Study RNA Catalysis*

In addition, there were eighty-six poster papers on a wide variety of topics. All together, there were 144 attendees from fifteen states, Canada and Australia.

Dirac Award Presentation

The first Dirac Award for Outstanding Graduate Research in Theoretical Chemistry was presented to Jason D. Thompson (University of Minnesota) for his paper "Reactions of Hydroxide with Chlorinated Hydrocarbons." His advisors are Christopher Cramer and Donald Truhlar (both from the Department of Chemistry, University of Minnesota). Jason presented the details of his research findings at the Dirac Award Lecture.

The Dirac Award is named after Nobel Laureate Paul Dirac who provided a foundation for much of the current research in theoretical chemistry.

The Supercomputing Institute would like to thank the Dirac Award Committee for the review of thirty-six abstracts, submitted for competitive review. The committee consisted of: James Skinner (University of Wisconsin, chair), J. Daniel Gezelter (University of Notre Dame), Lawrence B. Harding (Argonne National Laboratory), and Anne B. McCoy (The Ohio State University).

James Skinner from the University of Wisconsin at Madison presented statistical mechanical research on liquids and chaired the Dirac Award Committee.

Sundeep Rayat of the University of Missouri at Columbia enjoyed the poster presentations.

Left to right: Christopher Cramer, Jason Thompson holding the Dirac Award, and Donald Truhlar from the Department of Chemistry, University of Minnesota.

Visual Processing of Natural Images Symposium

On April 5th and 6th, 2002, the Computational Neuroscience Program will host a symposium on the Visual Processing of Natural Images: Theory, Psychophysics, Physiology, and Imaging.

Within less than a decade of the inception of information theory in the late 1940s, a number of scientists proposed that information theory could provide a link between environmental statistics and neural processing through efficient coding. Scientists theorized that the brain processes retinal images in terms of codes that maximize information transfer about the world despite sensory noise and that it does this by exploiting the statistics of natural images. Apart from a handful of subsequent studies in the following decades, it wasn't until the 1990's that theoretical developments in statistical modeling and computation were brought together to analyze high-dimensional image data sets, model these data, and propose quantitative neural models of visual processing. Comparisons with neural data have shown that several fundamental properties of the visual system (at both the retinal and cortical levels) can be understood in terms of adaptation to the statistical properties of the images received.

This symposium will bring together interdisciplinary research representing theoretical, neurophysiological, brain imaging, and psycho-physical approaches to the problem of visual processing of natural images. A key goal will be the discussion of extensions of this perspective to understanding higher level visual processing.

For further information and invited a list of speakers, please visit the symposium website at: www.compneuro.umn.edu/symposia.html, or contact the program organizers: Daniel Kersten (Chair), Sheng He, Paul Schrater, Gordon Legge, Cheryl Olman, Sing-Hang Cheung, Tom Carlson, and Kathleen Clinton, 612-625-8424.

Supercomputing Institute to Co-Sponsor Mini-symposium on Computational Chemistry at the Interface

The Supercomputing Institute will co-sponsor a mini-symposium as part of the 34th Great Lakes Regional Meeting, Chemistry at the Interface, to be held June 2-4, 2002, at the University of Minnesota in Minneapolis.

Chemistry at the Interface will highlight the exciting research being performed at the nexus between traditional subdisciplines and emphasize the impact that chemistry has on biology, the environment, and future technologies. Symposia on environmental chemistry, chemical biology, and chemistry of nanostructured materials will focus on experimental approaches. The Supercomputing Institute will co-sponsor Computational Chemistry at the Interface (June 3-4), highlighting computational approaches to problems from the same three symposia areas cited above.

Speakers will include William Arnold (University of Minnesota), Quiang Cui (University of Wisconsin), Ron Elber (Cornell University), Phil Gschwend (Massachusetts Institute of Technology), Sharon Hammes-Schiffer (Pennsylvania State University), Eric Patterson (Truman State University), Judith Perlinger (Michigan Technical University), Mark A. Ratner (Northwestern University), Paul Tratnyek (Oregon Health and Science University), and Olaf Wiest (Notre Dame).

Full information about this program is available at: www.chem.umn.edu/glrm. **Advanced registration closes on May 13, 2002.**

For questions about the program, please contact: William B. Tolman, University of Minnesota, tolman@chem.umn.edu, 612-625-4061.

Computational Neuroscience Program Hosts NSF-IGERT Site Visit and Plans a Symposium

The University of Minnesota Computational Neuroscience Graduate Program is sponsored by the Minnesota Supercomputing Institute and the Neuroscience Department and is supported in part by the National Science Foundation Integrative Graduate Education and Traineeship (IGERT) Program. The program introduces students with diverse biological and quantitative backgrounds to the challenges of complex phenomena in the neurosciences, and it fosters interdisciplinary training and research efforts toward meeting these challenges. A central problem in neuroscience concerns the modeling, representation, and processing of complex information. Areas of research include molecular modeling of receptors, ion channels and neurotransmitters, imaging and eigenvalue problems, single neuron models, motor control neurophysiology, modeling visual information processing and perception, neural networks and evolutionary algorithms, and problems in information flow.

As part of the NSF-IGERT program, Jerry Hipps, Nada Rayyes, Laurence Maloney, and Karen Sigvardt conducted a site visit to the Computational Neuroscience Program in October of 2001. Jerry Hipps and Nada Rayyes are from WestEd, a non-profit social policy research firm. Laurence Maloney is from the Center for Neural Science, New York University where he is a faculty member in the Department of Psychology. Karen Sigvardt chairs the Center for Neuroscience at the University of California-Davis and is a faculty member in the Department of Neurology.

Site visitors Laurence Maloney, New York University, Karen Sigvardt, University of California-Davis, and Nada Rayyes and Jerry Hipps, West Ed.

Computational Neuroscience Program Director, Timothy Ebner opened the program with an overview of the Computational Neuroscience Program. John Soechting (Director of Graduate Studies in Neuroscience), David Ferguson (Director of Graduate Studies in Scientific Computation), and Donald Truhlar (Co-Director of the Computational Neuroscience Program and Director of the Supercomputing Institute) presented overviews of coordinating programs. The program continued with the following student presentations.

John P. Clark discussed "The Role of HIV Transactivation Protein (Tat) in the Neuropathogenesis of the Circadian Clock." Clark and his advisor, Jian Ding of the Department of Medicine have carried out research that suggests that the HIV-1 protein, transactivation of transcription, induces glutamate receptor-mediated alterations in the circadian rhythms in a time-dependent and dose-dependent fashion.

Jadin Jackson's presentation, "Coherency Analysis of Head Direction Cell Model," described work carried out with his advisor David Redish of the Department of Neuroscience. They showed that coherency is a mathematically and statistically justified, robust measure of the validity of any value

reconstructed from any neuronal ensemble; it detects critical changes in state that reconstruction does not.

Cheryl Olman discussed the "Retinotopic Mapping in Cat Primary Visual Cortex: An fMRI Study." Cheryl and her advisor, Daniel Kersten of the Department of Psychology, discussed on-going studies at the University of Minnesota Center for Magnetic Resonance Research. These studies use high-field magnetic resonance imaging technology to localize brain activity in response to visual stimuli, thereby generating maps which are in agreement with single-electrode electrophysiological data. *This data can be acquired simultaneously across large regions of the brain through this non-invasive technology.

Eric Stevens discussed "D-Serine as a Co-Agonist at NMDA Receptors in the Vertebrate Retina." He explained that d-Serine potentiates inward currents in retinal ganglion cells, both at rest and during a light response, and that this increase in inward current is blocked by applying NMDA (*N*-methyl-d-aspartic acid) antagonists. His advisor is Robert Miller of the Department of Neuro-science and Department of Ophthalmology.

Thomas Naselaris discussed the "Ongoing Studies of Directional Mapping in the Motor Cortex." Thomas and his advisor, Apostolos Georgopoulos of the Department of Neuroscience and Department of Neurology, used artificial neural networks to transform the spiking activity of neurons into a control signal for a neuroprosthetic device.

The Computational Neuroscience Program is also planning a symposium, **Visual Processing of Natural Images: Theory, Psychophysics, Physiology, and Imaging** for April 5-6, 2002.

Computational Neuroscience Program Director, Timothy Ebner welcomed the site visitors and provided an overview of the program.

Cheryl Olman and Thomas Naselaris, Department of Neuroscience, gave presentations for the site visit.

*This data can be acquired simultaneously across large regions of the brain through this non-invasive technology.

2001 Undergraduate Summer Interns

Last summer, twenty-one undergraduate student researchers served ten-week internship appointments at the Supercomputing Institute. The students were selected from seventy-three applicants nationwide. The students performed research in close collaboration with faculty investigators and their research groups.

Currently in its eleventh year, the Supercomputing Institute Summer Internship Program promotes undergraduate involvement in ongoing and new research. Areas of study include scientific computing, digital technology, visualization in the physical, medical, and social sciences, and engineering, as well as software development for scientific computing and graphics in these areas. The program provides an opportunity for a challenging and enriching educational experience for undergraduate students interested in pursuing graduate or professional education and research in scientific computing and/or graphics.

During the summer, interns participated in Institute-sponsored tutorials specific to high-performance computing. Towards the end of the summer, the interns presented talks open to the entire research community that allowed them to share their work and gain experience making scientific presentations.

Left to right: Dawn Schafer, Clair Chisolm, and Victoria Bedell enjoy the program's opening activities.

Project Descriptions

Anthony Anderson, majoring in Chemical Engineering and Mathematics at the University of Minnesota, has been working under the supervision of Dr. Vittorio Cristini and Professor Christopher Macosko (Department of Chemical Engineering and Materials Science), and Professor John Lowengrub (School of Mathematics). Anthony developed adaptive three-dimensional numerical simulations of microstructured materials, with applications to multiphase polymeric flow as well as to biosystems such as tumors and their tissue environment. The main focus of Anthony's work was on the development of Fortran routines for volume mesh reconstruction, to be employed on unstructured meshes of tetrahedra. The goal of the adaptive strategy was to achieve a mesh distribution that resolves the relevant length scales in the specific problem with prescribed accuracy. This involves three distinct steps: 1) dynamic equilibration of the marker node positions based on an analogy to a physical system of springs; 2) refinement/coarsening via node addition and subtraction; 3) mesh reconnection via edge swapping to achieve nearly equilateral discretization. Anthony made significant progress on all of these steps, and completed routines for mesh equilibration and refinement which are now being tested.

Majoring in Computer Science at the University of Minnesota, **Abdul Bahar** worked with Professor Douglas Ohlendorf (Department of Biochemistry, Molecular Biology and Biophysics). During the summer, Abdul wrote a Perl script (for a UNIX system)

Michael Garrels from Case Western Reserve University enjoyed the Wednesday luncheons.

to automate map generation procedures. After giving it only one protein database file as input, his program generated maps, mask, and electron density files. This helped his research group save time by not importing the output of other procedures manually. He wrote procedures to generate identity matrices, multiply matrices, inverting 3 × 3 matrices, and using Cramers' rule to solve linear equations. Abdul also assisted in furthering the implementation of the Gaussian Elimination to solve linear equations.

A Biochemistry major from Bethel College, **Victoria Bedell** worked with Professor Steven Kass (Department of Chemistry). Victoria worked on research that involved carrying out high-level calculations on zwitterionic compounds (i.e., molecules which have a positive and negative charge site). Since all twenty essential amino acids exist in their zwitterionic form in water over a wide pH range, learning about these species is essential to gain a better understanding of protein structure and function. More specifically, Victoria assisted in carrying out geometry optimizations and vibrational frequency analyses on a series of methyl pyridinium anions, radicals and conjugate acids.

Sarah Betterman, majoring in Chemical Engineering at the University of Minnesota, worked with Professor David Grant (Department of Pharmaceutics). Sarah's research involved working with the software package Cerius2 to determine crystal structures from powder diffraction data using a compound called warfarin sodium. This drug has been used as rat poison and an anticoagulant for many years, yet its crystal structure has never been solved. This research group is trying to predict the crystal structure in order to explain the compound's solid-state properties and chiral discrimination in drugs and other molecules.

Nenad Bjelogrlic, majoring in Aerospace Engineering at the University of Minnesota, worked with Professor Fernando Porté-Agel (St. Anthony Falls Laboratory and Department of Civil Engineering). Nenad worked on a project that used an existing large-eddy simulation (LES) code to study the three-dimensional unsteady turbulent transport of heat, water vapor and pollutants in the atmospheric boundary layer (lowest part of the atmosphere, in direct interaction with the land surface). AMIRA and Iris Explorer were incorporated in the LES code, and the visualization process was automated. These tools were then used to visualize the dynamics of the atmospheric flow. This information was used by Porté-Agel's research group to identify and study the effects of different factors, such as, land surface heterogeneity and solar radiation on the transport rates. Nenad continues to work with the group on a web-based display of the visualizations (see: LES.safl.org).

Adam Butensky-Bartlett, majoring in Integrated Science/Biophysics at Northwestern University worked with Professor David Thomas (Department of Biochemistry, Molecular Biology and Biophysics). Adam's major research activity focused on simulation of Electron Paramagnetic

Resonance (EPR) spectra from molecular dynamics trajectories, with a goal of accurately simulating an EPR spectrum. EPR is a technique that studies the structural change of proteins (specifically the muscle proteins myosin, actin and the calcium pump) via the attachment of a spin-label to natural or artificially mutated cysteine residues. The result of this experiment was a graph (in frequency space) demonstrating the resonant frequencies of the spin-label, which vary between different cysteine attachment sites and are characteristic of the probe's local environment.

Mira Chaurushiyan, a Biology major at Carleton College, worked with Professor William Gleason (Department of Laboratory Medicine and Pathology). Mira worked in two major areas of research: the parallelization of protein database search algorithms, and the use of NAMD/VMD, an interactive molecular dynamics simulation package. NAMD is a parallel, object-oriented molecular dynamics code designed for high performance simulation of large, biomolecular systems, and was developed by the Theoretical Biophysics Group at the Beckman Institute at the University of Illinois. Dr. Gleason's research group uses Lutefisk, SEAQUEST, and other software to generate lists of potential peptide fragment sequences from experimental mass spectral data. Parallel versions of CIDentify (a protein database search program) then is used to search for these possible fragments in a database of known proteins to determine if they are present in any previously sequenced proteins. Using Message Passing Interface, parallel versions have been run on multiple processors of the SGI Origin and the 32-processor Netfinity Linux cluster at the Supercomputer Institute. Benchmark results indicate that a Linux cluster (on the order of eight processors) could be used, both for the software package that does this database search, and for the control of a mass spectrometer. If the potential sequences for a particular peptide fragment were found to not match any sequence in the protein database, and if this determination were made quickly enough, the machine searching the database could also control and modify the experiment automatically to obtain more information about the fragment.

University of Tuscaloosa Chemistry major **Claire Chisolm** worked with Professor David Thomas (Department of Biochemistry, Molecular Biology and Biophysics). Claire worked with Dr. Thomas's research group on Electron Paramagnetic Resonance (EPR) simulation from molecular dynamics trajectories, and was primarily involved with creating models of a spin-label that the lab regularly attaches to samples in order to run EPR spectroscopy. She used the InsightII/Discover software to build a molecule and optimize its structure. In addition, Claire worked on the actual EPR simulation program. The goal was to be able to create a simulated EPR spectrum from molecular dynamics trajectory data, and have it correlate to the experimental data. Her portion of this project was to code a Fast Fourier Transform routine in C in order to transform the magnetization trajectories (calculated from molecular dynamics data) into EPR spectra. Claire and Dr. Thomas' research group found that it is possible to directly

Below: Zachary Garbow and Samuel Stechmann discuss their research while enjoying one of the program's luncheons.

compare experimental and simulated EPR results, increasing clarity and understanding of the experimental results.

Interns **Jedediah Deitrick** (majoring in Computer Engineering at Kansas State University) and **Peter Holm** (majoring in Computer Engineering and Mathematics at Iowa State University) worked with Professor David Lilja (Department of Electrical and Computer Engineering). Both students spent their internship rewriting computer performance benchmark programs from the SPEC2000 benchmark suite. They used profiling tools to determine the function call patterns of the programs, identified loops that could be parallized (if any), and rewrote the code using the machine instructions for the superthreaded processor (a new computer architecture under development in Professor Lilja's group). Jedediah and Peter tested their parallel code using the simulator for the superthreaded processor. Once the parallel code was running correctly, they examined how much faster their parallel code ran (as compared to the original code) by looking at the instructions executed per cycle and other performance metrics. The work that Jedediah and Peter conducted during their internship will be incorporated into publications produced over the next year by Professor Lilja's research group.

Zachary Garbow, majoring in Computer Science from the University of Minnesota, carried out data mining research with Professor David Yuen (Department of Geology and Geophysics). Data mining is a research approach used to extract relevant data from particular locations in much larger data sets in both 2-D and 3-D. Zachary used an assortment of computer languages to develop graphical user interfaces in the form of Java applets, thus allowing users to interact in a client/server paradigm. By implementing web-based applications for data mining in geophysical data they have shown how data mining can effectively parse massive data sets to display results that are easy to understand and analyze. Their methods provide a new way of interrogating various forms of geophysical data and visualize the results in a fast and efficient manner.

Above: Sarah Betterman, Benjamin Langmead, Adam Butensky-Bartlett, and Nicholas Olson discuss one of the summer's tutorials.

Michael Garrels, majoring in Materials Science and Engineering at Case Western Reserve University, worked with Professor Woods Halley (Department of Physics). Michael studied ion conduction in amorphous polymeric electrolytes by conducting a classical simulation of the resonant frequencies of the triflouromethanesulfonate (triflate) ion. Modeling the atoms as balls and the bonds as springs, he used a harmonic potential in internal coordinates and expanded and translated it into Euclidean displacement coordinates. Michael wrote code that randomly varied the values of spring constants and compared the spectrum produced to the experimentally observed spectrum. Michael then chose the parameters, accordingly.

Majoring in Computer Science at Princeton University, **Jerome Hauser** worked with Professor Shir Ramaswamy (Department of Wood and Paper Science). Jerome worked on streamlining the image analysis program that they have developed for visualizing and characterizing the three-dimensional (3-D) structure of porous media, and also helped develop user documentation for the image analysis software. Using the new systematic procedure and user

documentation, he analyzed the 3-D structure of tissue and towel samples and then compared the results with other samples of different structure. He also worked on modifying another program to characterize the 3-D structure of porous materials using novel parameters, namely node density, coordination number and bond length distribution. Jerome also helped analyze the internal structure of a polymeric carrier fabric used in paper manufacturing using x-ray tomography images and the above mentioned image analysis program. For example, he calculated the average diameter of the machine direction and cross-machine direction polymeric fabric strands and then compared them to physical measurements using a microscope. He found out that the results from x-ray tomography and image analysis compared exceptionally well with less than 3 percent error. The image analysis system that they have developed uses a number of MSI resources, including the IBM SP supercomputer, with codes written in C++, MATLAB, etc. Jerome also organized the format making it suitable for scientific presentations.

Eric Johnson, majoring in Biomedical Engineering at the University of Minnesota worked with Professor William Gleason (Department of Laboratory Medicine and Pathology). Eric worked in two major areas: parallelization of CIDentify from the Lutefisk/CIDentify software package, and using a molecular dynamics simulation and visualization (NAMD/VMD) software package in interactive molecular dynamics simulations. The NAMD/VMD is used because of its interactive capability. It is possible for large-scale molecular dynamics calculations to be carried out by NAMD on the supercomputer, while visualization is accomplished on a local machine by VMD without the need for special graphics pipes. Not only can the physical results of the calculations be observed as they occur, the user can intervene by introducing forces or moving molecules and then immediately view the results. To investigate this software as a tool for computation and visualization Eric looked at Vascular Endothelial Growth Factor (VEGF). After becoming acquainted with the NAMD/VMD program, he learned to use the XPLOR software package to generate protein structure files from structures found in the protein database (PDB), obtained through x-ray crystallography and nuclear magnetic resonance spectroscopy. These two types of files, when properly created and modified can be combined with existing protein topology and parameter files to run dynamic simulations. Eric used this process to simulate the binding of VEGF to a receptor and to an antibody fragment. The dynamic simulation gives additional insight into the binding, supports the argument that the dynamic model created is sound, and the structure contained in the PDB accurately portrays the actual binding mode. Eric also worked on developing topology and parameter files for simulating the dynamic behavior of a heparin model.

Below: Jedediah Deitrick, Peter Holm, AJ Klein Osowksi, and Abdul Bahar await the beginning of a tutorial.

Majoring in Computer Science at Columbia University, **Benjamin Langmead** worked with Professor Yousef Saad (Department of Computer Science and Engineering). Benjamin's work was geared toward enhancing and improving SPMATH, a package developed entirely with three under-

graduate interns from MSI. SPMATH is a package to help solve sparse matrix problems (see also, our article Improving the Efficiency of Sparse Matrix Storage, page 6). Benjamin developed a new graphics interface based on the Total Command Language/Toolkit (TCL/TK). He also improved portability using Autoconf configure scripts, fixed a few computational bugs and improved functionality. As a result of Benjamin's work, this package has now been made available to the public (see: www.cs.umn.edu/~saad/software).

John O'Leary, majoring in Computer Science and Biology at the University of Chicago, worked with Leonard Banaszak (Department of Biochemistry, Molecular Biology and Biophysics). John worked primarily on using genomic data to understand protein structures. Protein structure determines protein function, but how this occurs it not yet fully understood. John focused on using the large number of protein sequences in the National Center for Biotechnology's database as a tool to more clearly understand the role played by various parts of the structures of the enzymes in the tricarboxylic acid cycle. Primarily, John did a literature survey on both protein structure and common bioinformatics tools, and then ran sequence and structure databases to analyze the data. He used Perl programming to parse and manage the large amount of data that was generated through database searches. This resulted in the construction of a module that, after the entry of a protein name, makes multiple web requests in order to gather and separate out only the appropriate data for running a multiple sequence alignment. Multiple sequence alignments were determined using CustalX, and after their analysis with another Perl script, diagrams were made (using InsightII, RasMol, and Molscript) of the structures with conserved residues highlighted. Eventually, by using visualization software it can be discovered not only which residues are crucial to enzymatic function, but also *why* they are crucial.

Above: Eric Johnson and Mira Chaurushiyan discuss the program during a luncheon break.

Mariah Olson, majoring in Computer Science and Biology at University of Minnesota, Duluth worked with Professor David Levitt (Department of Physiology). Mariah worked on the development of a web-based database that could be used to carry out intelligent searches of the structures and sequences of antibodies and the peptides that they bind. She combined several different databases into one relational SQL database. This required extensive use of Perl scripts. Finally, Mariah began the development of an interactive web site to allow general use of these databases.

Nicholas Olson, majoring in Electrical Engineering at University of Maryland, College Park, worked with Professor David Yuen (Department of Geology and Geophysics). Nicholas worked on a design map for data mining that could work over the Internet. This program would display an image developed from previous data, and, after placing a grid over the image, the program would provide the average, standard deviation and a histogram for each square within the grid. By enlarging or shrinking the grid the program will change the range of values in the histogram.

Jonathan Othmer, majoring in Mathematics and Music at Williams College

Jerome Hauser of Princeton University (left) and John O'Leary from the University of Chicago.

(Williamstown, Massachusetts) worked with Professor Heinz Stefan (St. Anthony Falls Laboratory and Department of Civil Engineering). Jonathan joined Dr. Stefan's research group and did an analysis of a large stream temperature database for stream gauging stations throughout the United States. Initially, they looked for trends and patterns in the data relating to geographic distributions and record length. Then looking for a statistical upper bound on stream temperatures, they tried to improve upon previous work done on this topic. This is of interest to determine how far stream temperatures can rise if the climate warms. The physics of heat exchange suggest that stream water temperatures do not rise indefinitely. This is of great importance for stream water quality and biological habitat. Jonathan is continuing his work on a linearization method for estimated upper bounds on temperature. The best estimates of the upper bound for stream temperatures were presented in histogram and map format.

Rice University Computer Science major, **William Ryan** worked with Professor Thomas Jones (Department of Astronomy). William's work concentrated on two graphical user interfaces (GUIs) used by astronomy researchers. The first program is used to position the viewing space and setting the input parameters to a synthetic observation of a radio galaxy. William succeeded in having this program interface with the Fortran program, running the observation. The second GUI performs numerous operations on data generated by the previously mentioned synthetic observation program. Among these, the most complicated was the gathering of data along a line-of-sight through the two-dimensional image representation of three-dimension. This interprocess communication with existing Fortran code was then modified. William also did research analyzing the polarization of synthetic data, primarily to observe the orientation of magnetic fields, but also to look at Faraday rotation.

Dawn Schafer, majoring in Biochemistry at Bethel College worked in the laboratory of Professor Ian Armitage (Department of Biochemistry, Molecular Biology and Biophysics). After an extensive literature review of nuclear magnetic resonance (NMR), Dawn worked on the basic theory and experimental aspects behind one- and two-dimensional NMR, using Varian software (6.1B VNMR) and NMR instrumentation to acquire, process and analyze data and create high-quality spectra. Dawn found that the most challenging aspect was associated with shimming or obtaining a homogeneous magnetic field around her sample. With the assistance of NMR facility personnel, Dr. Beverly Ostrowski, she learned to acquire one-dimensional, and the more challenging, two-dimensional spectra, specifically Correlation

Spectroscopy, Total Correlation Spectroscopy, and Nuclear Overhauser Effect Spectroscopy on her protein sample.

Samuel Stechmann, majoring in Physics, Applied Mathematics and Chemistry at the University of St. Thomas worked with Professor Donald Truhlar and graduate student Ahren Jasper in the Department of Chemistry. Samuel worked on a time-uncertainty method for enabling classically forbidden electronic transitions in trajectory surface hopping calculations. He worked on a nonadiabatic trajectory (NAT) code that is written in Fortran and is used to simulate quantum mechanical photochemical reactions using semiclassical approximations. With such semiclassical approximations, the electrons are treated using quantum mechanics and the nuclei are dealt with using classical mechanics. The quantum mechanical electronic motion gives rise to potential energy surfaces over which the nuclei are propagated quasi-classically. Using this semiclassical approach simplifies the calculations, thereby reducing the expense of the simulation as compared to full quantum mechanics. Therefore, the development of these semiclassical methods is important for simulations on larger chemical systems for which quantum mechanical calculations are too expensive to carry out. They used the results (the electronically nonadiabatic transition probabilities and vibrational and rotational moment of the products) of quantum mechanical simulations on small (atom-diatom) systems as bases of comparison for the various prospective semiclassical methods.

Summer 2002 Undergraduate Internship Program

The Supercomputing Institute is pleased to announce its Undergraduate Internship Program for Summer 2002. Summer appointments will be full-time, ten-week appointments, and will run from June 10th through August 16th, 2002. A student interested in becoming an intern must be an undergraduate student during the internship to be eligible and must be a citizen or permanent resident of the United States or its possessions.

All applications are evaluated competitively based on the qualifications of the applicant and the availability of a suitable project. Applicants should review the research projects list and choose projects in which they are interested, although they may be offered other projects due to availability.

Further information, application forms, and project lists are available on the Internet at:

www.msi.umn.edu/general/Programs/uip/summer02.html

Application form and project lists are also available by contacting:

Undergraduate Internship Coordinator
University of Minnesota
Supercomputing Institute
1200 Washington Avenue South
Minneapolis, Minnesota 55415-1227

Phone: (612) 624-2330
Email: uip@msi.umn.edu

The application deadline is February 28.

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