Our Mission

The Supercomputing Institute for Digital Simulation and Advanced Computation is an interdisciplinary research program spanning all colleges of the University of Minnesota. The Supercomputing Institute provides supercomputing resources and user support to faculty and students and is a linchpin program in the University's broad-based digital technology effort. The mission of the Supercomputing Institute is supercomputing research. This includes all aspects of high-performance computing and scientific modeling and simulation as well as graphics, visualization, and high-performance network communications. Supercomputing research is defined broadly to include a variety of research activities from many disciplines. This research involves the use of high-performance computing environments to address problems in science and engineering that could not otherwise be attempted. Such efforts often result in domain-specific algorithms and codes that exploit the available computing environments as well as visualization techniques to enhance insight, make displays more informative, and add multimedia value to communications and work environments. In many cases, these research activities may involve research aimed at the design or evaluation of high-performance computing hardware, operating systems, networking, and general-purpose algorithms and software.

The Supercomputing Institute's resources are available to researchers at the University of Minnesota and other post-secondary educational institutions in the State of Minnesota. In addition, the Supercomputing Institute organizes and hosts symposia, workshops, and seminars and coordinates other educational and collaborative activities to promote supercomputing research, increase university-industry collaboration, and promote technology transfer.

Supercomputing Resources

In 1981, the University of Minnesota was the first American University to acquire a supercomputer (a Cray-1B). The Supercomputing Institute was created in 1984 to provide leading edge high-performance computing resources to the University of Minnesota's research community. These resources have included a Cray-2, an ETA 10, a Cray X-MP, an IBM 3090, a Cray M90, a Cray T3D, a twelve-processor Cray C90, and a Cray T3E-900. These resources were provided to the Supercomputing Institute by Network Computing Services (formerly Minnesota Supercomputer Center, Inc., or MSC Inc.). Beginning on July 1, 1998, the Institute began providing services on its own supercomputers.

Building upon the strong tradition of providing University of Minnesota researchers with leading edge high-performance computing technologies and diversified programs that complement these technologies, the Supercomputing Institute acquired in May 1998 a 256-processor IBM SP with 192 GB of memory. This IBM SP supercomputer is a 64-node machine with four 332 MHz 604e processors and 3 GB of memory on each node.

The Supercomputing Institute also offers its researchers access to a 128-processor SGI Origin 2000 R10000 supercomputer which has a clock speed of 195 MHz and a total of 64 GB of memory. In June,

the Institute upgraded 48 processors of this machine to R12000 technology. The upgraded processors have a total of 36 GB of memory. Fourteen more R12000 processors with 14 GB more memory are scheduled for delivery for a total of 62 R12000 processors with 50 GB of memory. The R12000 processor, which has a clock speed of 300 MHz, is estimated to be 1.7 times faster than the R10000 processor.

With the arrival of 80 WinterHawk nodes in May 1999, the Institute acquired the lastest SP technology from IBM. Each of the WinterHawk nodes contains two 200 MHz Power3 processors sharing 1 GB of memory for a total of 160 WinterHawk processors. In October 1999, the IBM SP will be expanded to include 17 NightHawk nodes. Each node will contain 4 Power3 processors sharing 16 GB of memory for a total of 68 NightHawk processors. When fully configured, the IBM SP will contain 228 processors and 352 GB of memory. We anticipate that the IBM SP will be 2.5 times faster than the current IBM SP that contains 64 Silvernodes.The IBM supercomputer resources are available in coordination with the IBM Shared University Research (SUR) parthership.

The total amount of disk available to users of the IBM SP systems is currently 1.5 Terabytes.

Current Resources

The supercomputing resources are located at the Supercomputing Institute's facilities in the Minnesota Technology Corridor at the edge of the West Bank of the Minneapolis Campus of the University.

In addition to IBM SP and SGI Origin 2000 supercomputers housed at the Supercomputing Institute, the Supercomputing Institute offers IBM SP resources through its IBM East Bank Laboratory. This laboratory, which is co-managed by the Supercomputing Institute and the Computer Science and Engineering Department, includes 72 processors with 36.5 GB of memory and 500 GB of disk.

These IBM and SGI supercomputers offer the Supercomputing Institute's researchers access to state-of-the-art high-performance computing technology. In addition, the Supercomputing Institute is continuing its commitment to a diversified array of computing laboratories, collaborations, and programs. These include the Basic Sciences Computing Laboratory, the Scientific Development and Visualization Laboratory, the Medicinal Chemistry-Supercomputing Institute Visualization/Workstation Laboratory, and interdisciplinary Ph.D. programs in Scientific Computing and Computational Neuroscience.

Laboratories of the Supercomputing Institute

IBM Shared University Reserach East Bank Laboratory

The IBM SUR East Bank Laboratory is a cooperative research effort in scientific and parallel computing between the University of Minnesota and IBM. The project is managed under the auspices of the IBM Shared University Research (SUR) program by the Computer Science Department, the Office of Information Technology, and the Supercomputing Institute. This program makes a cluster of IBM RS/6000 workstations and an SP POWERparallel system available to University of Minnesota

researchers for research on system software, communications, parallel algorithms, and computational science applications.

As part of the program, the University has an IBM RS/6000 Cluster, which consists of four subsystems: an 8-node RS6000 workstation subcluster, a 16-node SP supercomputer, a 4-node, 32-processor SMP supercomputer, and a 4-node, 16-processor SMP Silvernode supercomputer. The total number of processors available is 72 and the total amount of memory is 36.5 GB. In addition, there are several machines that support the RS6000 Cluster. These include an RS/6000 G30 that acts as a file server, an RS/6000 model 380 and an RS/6000 43P for staff use, and the SP control workstation. These computers are housed in the Computer Science building.

The SUR Cluster is supported by IBM, the University of Minnesota Supercomputing Institute, the National Science Foundation through the Directorate for Computer and Information Science and Engineering, the Office of Information Technology and the Department of Computer Science at the University of Minnesota, and various University of Minnesota researchers through individual research grants.

Basic Sciences Computing Laboratory

In 1996ï¿½97, the Supercomputing Institute established the Supercomputing Institute Basic Sciences Computing Laboratory in the Nils Hasselmo Hall located on the East Bank campus of the University of Minnesota. The laboratory provides high-performance workstations and visualization equipment to enhance the research capabilities of the University community. The facility occupies approximately 1700 square feet that includes a workstation room, video/graphics room, machine room, and two offices. The laboratory houses state-of-the-art computing platforms and graphics workstations including five Silicon Graphics Indigo2 Solid Impact R10000 workstations, a Silicon Graphics Challenge XL with four 150 megahertz R4400 processors, two SGI Octane SSI workstations, one SGI Octane MXE workstation, two SGI Octane SSEs, one SGI Onyx2, one IBM Intellistation, and a 32-processor Origin 2000 with 8 GB of memory.

The Supercomputing Institute provides technical support for these high-performance computing resources, and the laboratory is available to all University of Minnesota researchers.

Medicinal Chemistry-Supercomputing Institute Visualization/Workstation Laboratory

The Medicinal Chemistry-Supercomputing Institute Workstation/Visualization Laboratory is cosponsored by the Department of Medicinal Chemistry and the Supercomputing Institute. This laboratory is located in Weaver-Densford Hall and contains workstations that are used primarily for scientific visualization. This facility is available to all researchers who apply for and receive competitively reviewed supercomputing resource allocations. Access is also available by separate proposal for those researchers requiring workstation access only.

Scientific Development and Visualization Laboratory

The Supercomputing Institute's Scientific Development and Visualization Laboratory, which is located in the Supercomputing Institute's facilities in the Supercomputer Center Building, provides front-end equipment including Silicon Graphics workstations, Macintosh workstations, an Intellistation from IBM running Windows NT, a color scanner, a CD writer, a Silicon Graphics O2 workstation for the creation and manipulation of videos, and a Super-VHS VCR.

The Institute provides user support services for supercomputer-related research using these general-purpose systems. The computer resources and user support services of the Scientific Development and Visualization Laboratory are available to all researchers who apply for and receive competitively reviewed supercomputer resource allocations. Access is also available by separate proposal for those researchers requiring workstation access only.

National Center for Supercomputing Applications Resources

The Supercomputing Institute is also coordinating the allocation of National Center for Supercomputing Applications (NCSA) SGI Origin 2000 resources to University of Minnesota faculty researchers. These resources are being made available through the Committee on Institutional Cooperation (an academic consortium of Big Ten Universities and the University of Chicago).

The goal of all of these efforts is to foster state-of-the-art research, interdisciplinary collaboration, and university/industry collaboration by providing Minnesota researchers with access to advanced facilities for digital computing, visualization, and networking.

Collaborative Projects

IBM Shared University Research Workstation Award Program

IBM, through its Shared University Research Program, has made available to the University of Minnesota Supercomputing Institute, a number of IBM RS/6000 and Intellistation workstations. These workstations have been awarded through a competitive grant program administered by the Supercomputing Institute. The Supercomputing Institute and the Computer Science and Engineering Department provide hardware and system support and user and parallel programming support.

The Intellistation workstations are Z Pro Windows NT machines with Pentium II 450 MHz processors, 256 MB RAM, 9.1 GB hard drives, 32 way CD readers, Intergraph Intense Graphics 3400 video cards, and 10/100 ethernet connections. The workstations have a 21ï¿½ monitor. The RS/6000 UNIX workstations contain two 332 MHz 604e processors, the same processor in the Silvernodes of the IBM SP and the GTX550P graphics adapter.

Laboratory for Computational Science and Engineering

The Supercomputing Institute partners with the Laboratory for Computational Science and Engineering (LCSE) in support of the LCSE's participation in the National Center for Supercomputing Applications (NCSA) National Computational Science Alliance, which has been funded by the National Science Foundation. Through this partnership, Supercomputing Institute researchers are able to participate in the LCSE program.

The LCSE encourages the participation of Supercomputing Institute researchers with applications that demonstrate or test new technologies under active development, applications requiring very large on-line data setsï¿½particularly if they must be accessed at very high bandwidth, applications requiring very high-resolution visualizationsï¿½particularly if image animations are needed, and distributed

computing applications with tight coupling of computing resources on a fast network are also encouraged.

Scientific Computation Graduate Program

The graduate degree program in scientific computation encompasses course work and research on the fundamental principles necessary to use intensive computation to support research in the physical, biological, and social sciences and engineering. There is a special emphasis on research issues, state-of-the-art methods, and the application of these methods to outstanding problems in science, engineering, and other fields that use numerical analysis, symbolic and logic analysis, high-performance computing tools, parallel algorithms, supercomputing and heterogeneous networks, and visualization.

Scientific Computation is gradually emerging as an important field of its own in academia and industry. In the last decade, it has become clear that solving a given scientific problem often requires knowledge that straddles several disciplines. This interdisciplinary program provides a new combination of studies for solving today's scientific computational problems. It is a degree program that builds on the strength of existing programs at the University of Minnesota in formulating real problems based on the physical system or the traditional discipline, and it augments field-specific work relating to the mathematical and numerical modeling with state-of-the-art techniques for scientific computation in an integrated manner.

The Scientific Computation program offers Ph.D. and M.S. degrees.

Computational Neuroscience Graduate Program

This program introduces students with diverse biological and quantitative backgrounds to the challenges of complex phenomena in the neurosciences and fosters interdisciplinary training and research efforts toward meeting these challenges. Graduate Programs in Scientific Computation and Neuroscience are united with the Supercomputing Institute to provide a new paradigm for training graduate students interested in the physical, chemical, and computational sciences. This lowers the barriers to interdisciplinary research, provides opportunities for neuroscientists to pose problems to the quantitative sciences, and provides a catalyst for the cross-fertilization of the two disciplines.

Other Collaborators

In addition, the Supercomputing Institute collaborates with many other centers of the University of Minnesota. The Supercomputing Institute has cosponsored various research projects, symposia, and workshops with the Aerospace Engineering and Mechanics Department, Army High-Performance Computing Research Center, Institute of Medical Biotechnology, Biological Process Technology Institute, Brain Sciences Center, Center for Interfacial Engineering, Chemical Engineering and Materials Science Department, Computer Science and Engineering Department, Corrosion Research Center, Engineering Research Center for Plasma-Aided Manufacturing, Center for Transportation Studies, Institute of Human Genetics, Laboratory for Computational Science and Engineering, Institute for Mathematics and Its Applications, Limnological Research Center, Medicinal Chemistry Graduate Program, Particle Technology Laboratory, Advanced Bioscience Computing Center, Office of Information Technology, St. Anthony Falls Laboratory, Structural Biology Program, Scientific

Computation Graduate Program, and the Theoretical Physics Institute.

The Supercomputing Institute is also playing a central role in the University of Minnesota's digital technology initiative. This initiative includes technologies based on computers, electronics, and telecommunications. Key to this initiative is the renovation of Walter Library on the University's East Bank Campus into a Digital Technology Center. This renovation, which has been funded for $53.6 million, will keep the library's historic 1920s decor intact while revamping the interior to include state-of-the-art technology. The Supercomputing Institute will be one of the principal tenants of the Digital Technology Center. Completion of the renovation is scheduled for January 2001. An important part of the Ditigal Technology Initiative is the hiring of four senior faculty in computational biological sciences.

Other Programs

Supercomputing Institute Research Scholars

In addition to providing state-of-the-art supercomputing resources to the University of Minnesota research community, the Supercomputing Institute offers a Research Scholarship Program which provides grants to enhance the supercomputing research programs of University of Minnesota faculty. These grants, which are peer reviewed and competitively awarded, are for the support of research associates who work closely with Supercomputing Institute principal investigators on their research projects. Over the past ten years, 170 Supercomputing Institute Research Scholarships have been awarded. These Research Scholarships have provided an important opportunity for the creation and pursuit of research projects that might not have otherwise been attempted.

Supercomputing Institute Undergraduate Interns

The Supercomputing Institute's Undergraduate Internship 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 ten-week appointments, interns participate in Institute sponsored tutorials specific to high-performance computing and individual laboratory tours led by faculty members. To conclude the program, interns present talks that allow them to share their work with other researchers and to gain experience making scientific presentations. The program allows 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. The program has sponsored 340 interns in its ten years of existence.

Department Index

University of Minnesota--Duluth Campus

College of Science and Engineering

Department of Chemistry

Paul Kiprof
Paul Siders

Paul Kiprof, Principal Investigator

Silene Cycloaddition Reactions

Cycloaddition reactions with carbon compounds have been widely studied and have found wide use in organic synthesis. [2+2] cycloaddition reactionsï¿½including carbon-carbon multiple bondsï¿½are thermally forbidden but photochemically allowed. Still, there are several examples of thermal [2+2] cycloadditions involving radical or dipolar intermediates. An ab initio molecular orbital study of ring opening reactions of four membered carbon rings has been carried out recently. A major breakthrough was achieved when a diradial intermediate for the ring opening of cyclobutane could be observed directly. By way of contrast, cycloaddition reactions of analogous silicon systems were only recently discovered.

The transition states at the Hartree Fock level for cycloaddition reactions with carbon compounds have been found. Both MP2 (Møller-Plesset second order energy correction) level and Complete Active Space Self Consistent Field (CASSCF) calculation methods confirmed the transition state for the acetylene case. In the ethylene case, the MP2 level calculations confirmed the transition state, but CASSCF level calculations indicated the presence of a second order saddle point at the Hartree Fock geometry. This was a strong indication that the concerted pathway is doubtful for the ethylene case.

Alternative pathways that have a diradical intermediate for both cases and a silacyclopropylcarbene intermediate for the acetylene case are the focus of the current study. High level ab initio calculations are being used to study substituent effects on cycloaddition reactions on silenes. The high levels of treatment this requires makes use of GAUSSIAN and GAMESS.

Further study is being done on the multiple bonds of silicon with transition metals. Multiple bonds to transition metals are very common in the case of carbon, and their bonding is well understood. However, there is still a lack of understanding for multiple bonds in the case of siliconï¿½the most prominent examples being multiple bonds between silicon and transition metals in silylene complexes. Two classes of silylene complexes exist. The type I complexes have a bond that qualifies as a true double bond (in the classical sense). The type II complexes have the silicon atom stabilized with a donor molecule. This research is continuing calculations on both types of silylene complexes in the hope that differences in bonding will be revealed in calculations.

In order to study the differences of type I and type II silylene complexes, a model system was chosen that consists of a transition metal fragment Cr(CO)5 and a silylene or a base stabilized silylene respectively. Both molecules were refined by Hartree-Fock methods. It was found that the metal silicon distance strongly depends on the presence or absence of the Lewis base. In the case without a Lewis base, the bond is close to a double bond (2.30 Å). In the case where there is a Lewis base coordinated, the distance increases to 2.52 Å, corresponding to a single bond. Investigations at correlated levels of theory are currently being performed as are determinations of rotational barriers of the M-Si bond.

In addition, silylene complexes of the silylene 2 were optimized at the Hartree-Fock and MP2 levels of theory. In the case of a complex with Fe(CO)4, the silylene has two possible coordination sites to occupy, the axial and the equatorial position. Both geometries were considered in order to compare their energies. Using the MP2 method, more reasonable geometries can be obtained.

Research Group

Benjamin Lynch, Graduate Student Researcher
Kyle Riess, Undergraduate Student Researcher
Jonathan D. Thompson, Undergraduate Student Researcher

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Paul Siders, Principal Investigator

Ab Initio Molecular Modeling of Calcite Surfaces and Adsorption

Calcite (calcium carbonate) is the main component of limestone. Calcite surfaces are almost unrelaxed from slices through the bulk crystal and react rapidly with water and aqueous ions. Interaction of aquated ions with calcite surfaces leads to growth inhibition and concentric, sector, and intrasector zoning. Reactivity of carbonate growth surfaces is influenced by geometry of the surface and by solution species bound to the surface: hydroxide, water, hydrogen carbonate, carbonate, and metal ions in various stages of hydration. This research is theoretically characterizing, at the atomic level, the energetically favored species at the calcite surface that may be responsible for growth features.

Many carbonate crystals display concentric zoningï¿½nonhomogeneous distribution of minor and trace elements in bands parallel to growth surfaces. At least in some cases, zoning arises from surface-controlled kinetics rather than changing growth conditions. Minor and trace elements including Magnesium, Manganese, and Strontium also display concentration zoning in different growth sectors. Surface control related to different atomic configurations on different faces is likely. Shark Magnesium, Manganese, and Strontium zones have also been identified within sectors. It has been argued that such intrasector zoning is systematically related to the structure and orientation of steps and kink sites. Several ions slow calcite growth and inhibition by magnesium that has been thoroughly studied by distortion of the near-surface calcite lattice or slow dehydration of adsorbed magnesium.

Hydration of the surface and of adsorbing ions is important in calcite growth. Water is readily adsorbed onto calcite, but little is known about how water adsorbs at the atomic level. Candidates for the adsorbed form include hydroxide and protons bonded to calcium and carbonate or water attached through its oxygen atom to calcium with a hydrogen bond to a nearby carbonate.

This group has done preliminary embedded-cluster calculations for attachment of ions to CaCO3. For example, to model the kink sites on the 10 14 surface, they used (CaCO3)3, 5 Ca2+ core potentials and 121 point charges. Hartree-Fock method was used in gamess and the ALRICHS+* basis set. Modifications were made to accept point charges, and continuing changes were made to model kink sites on the 10 14 surface. Preliminary results indicated that a few hundred point charges are adequate, and it is possible to model adsorption on an embedded carbonate cluster, but considerable development work is still required. Development work underway includes identifying a smaller, yet reliable, basis set to reduce computation times. The number and location of point charges bears further study. Corrections are being made for electron correlation and basis set superposition errors.

The smaller basis set and embedding point charges are already being chosen and augmented. Calculations are also being extended from the 10 14 cleavage surface to the 10 12 and 01 12 surfaces. Hydration energies are being studied on the same terrace, step, and kink models used for cation binding studies. Finally, energies of protonated carbonate and hydroxylated calcium are compared to whole water attachment.

Research Group

Rachel Green, Graduate Student Researcher
John Podobinski, Undergraduate Student Researcher

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Department of Mathematics and Statistics

Harlan W. Stech

Harlan W. Stech, Principal Investigator

Hierarchical, Parallel Modeling Strategies for Simulating Plant Response to Environmental Stress

Computer simulation models provide key tools for synthesizing existing research information (predicting the behavior of complex biological systems) and identifying new research questions. Detailed mechanistic or process models have added advantagesï¿½they incorporate theoretical equations and can be used to make predictions outside the range of data used in model development. Individual-based process models add a further degree of biological realism to the models, but there are drawbacks to individual-based process models. Individual-based models do not account for processes operating in different temporal and spatial scales, they are not well-adapted to qualitative information, and they tend to be computationally intensive.

Recent advances in hierarchically-organized parallel computing provide fertile ground for biological modeling. Biological systems are generally hierarchical in nature and comprise processes that are inherently parallel. This project uses an established, object-oriented growth process model of Populus

as a platform for developing generalized hierarchical, parallel processing, and regulatory strategies for biological simulation models.

New algorithms are being developed to resolve problems of scaling, parallel computing, and regulation in simulating biological systems. The resulting models are used in conjunction with experimental work to test hypotheses on plant response to environmental stress. Specific work already underway includes development of a hierarchical, scalable, non-proprietary strategy for running object-oriented models in parallel across a distributed network of workstations, development of a heuristic regulatory system that directs model behavior, and use of the model in conjunction with experimental work to test hypotheses.

Overall, this project addresses an important current issue in computational biology. It generates heuristics and code for a field of individual based biological simulation modeling in the form of object-oriented, parallel processing algorithms that can be used to simulate other similar, self-generating biological processesï¿½a scalable, accessible simulation environment for heuristic or predictive purposes, an integration of object-oriented languages and a standardized threads library for use in a heterogeneous network; and an educational tool that represents a synthesis among mathematics, computer science, and biology.

The computational aspect involves a hierarchical, integrated approach that embeds an object-oriented computing paradigm within a parallel processing environment. The existing model is used as a platform for developing this approach. This computational component is coupled to an accessible graphical user interface for setting input parameters and for analyzing resultant model output. The software development is designed to maintain extensibility of the program, portability to different computational platforms and to various network configurations, independence from proprietary software products that would restrict distribution of the final product, and accessibility to scientists with varying degrees of computer experience along with students in biological sciences and mathematics programs.

Research Group

Kathleen McTavish, Graduate Student Researcher

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Department of Physics

John R. Hiller

John R. Hiller, Principal Investigator

Nonperturbative Analysis of Field Theories Quantized on the Light Cone

These researchers are investigating nonperturbative techniques for the analysis of quantum field theories. The techniques are based on light-cone coordinates where t + z/c is treated as the time coordinate for evolution of a system with the ordinary time t, a Cartesian spatial coordinate z, and the

speed of light c. The states of a theory are obtained from solution of an eigenvalue problem that couples the probability amplitudes (wave functions) for constituents via integral equations.

In the construction of solutions to these equations, infinities are encountered. These can be absorbed into redefinitions of the theoryï¿½s parameters. To do so in practice requires regulation of the infinities. One of the ways to accomplish this is the introduction of heavy particles with imaginary couplings that cancel the infinities in any physical quantity (Pauli-Villars regularization). In such a scheme, numerical calculations include the heavy particles as constituents; any unwanted effects are eliminated in a large-mass limit. All previous uses of this method were perturbative.

Implementation of this approach was successfully tested on an analytically soluble model and has now been extended to a more sophisticated model for which no analytic solution exists. This makes it capable to obtain explicit forms for wave functions in the valence sector and for any reasonable number of (virtual) constituents. The new IBM SP has allowed the number of discrete momentum states included in these calculations to be increased from 1.5 to 10.5 million.

For some field theories, structure of the vacuum receives important contributions from modes with zero longitudinal momentum. In particular, such modes can induce breaking of symmetries in the original theory so thatï¿½like a ferromagnetï¿½the ground state of the system has some asymmetry. One such theory, f4 in one space dimension, had been studied previously with inconclusive results coming from poor convergence. A new approach has now been developed and applied. The results indicate that the naive discretization of the light-cone integral equations does not capture the physics of the f4 vacuum. New formulations in the continuum are being explored.

In other theories, the inclusion of zero modes is important only for improved numerical convergence. The precise nature of this improvement is being studied. The most efficient means of including zero modes appears to be the addition of effective interactions between the other modes rather than explicit zero-mode occupation.

Research Group

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College of Agricultural, Food, and Environmental Sciences

Department of Biosystems and Agricultural Engineering

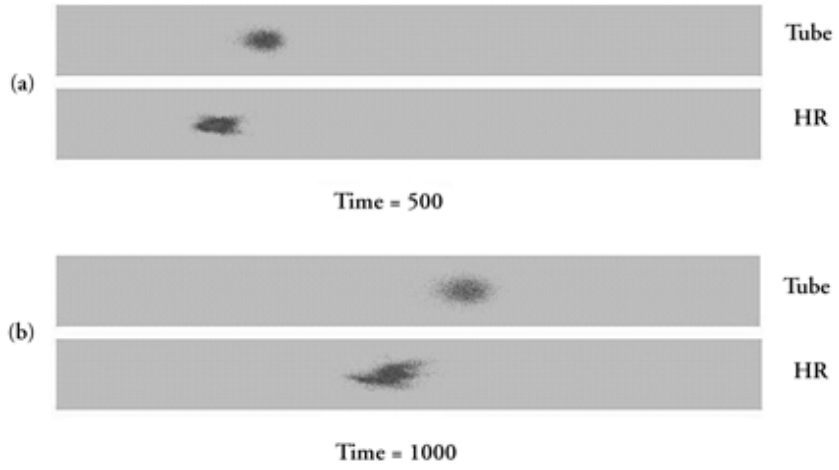
John L. Nieber

John L. Nieber, Associate Fellow

Simulation of Flow and Contaminant Transport with Biochemical Transformation in Variably Saturated Heterogeneous Porous Media

Simulation of flow and contaminant transport in heterogeneous porous media with degradation and biochemical transformation is the focus of this work. Three issues are central to the investigation. The first issue is dispersion in porous media. This issue needs to be quantified at different levels of flow field heterogeneity. The second issue is unstable wetting fronts. These are observed in unsaturated flow resulting from hysteresis and behavior at microscopic scales. There are still many questions awaiting resolution as to the factors that effect the inception and persistence of unstable fronts. The final issue deals with the behavior of solutes undergoing degradation and biochemical transformation. These processes are often nonlinear and are influenced by numerous spatially heterogeneous parameters and variables in the porous medium.

All of these issues result from the behavior of fluids as well as solutes at the molecular and microscopic scales. In order to resolve these issues, flow and transport processes have to be simulated for high-resolution flow and parameter fields. These simulations require dense numerical grids for the flows. Solute transport is being simulated using a particle method. The dynamics of biomass transport and the biochemical reaction processes are considered in the simulations along with the movement of the solute in the porous media. This requires massive computations that require a great deal of computer memory and processing time in order to be able to resolve variations in flow and concentration fields at very small scales. The code is now being parallelized to run more efficiently and save resources.



Concentration plumes at different times simulated with particle tracking using a high-resolution (HR) velocity field and dependent particle tracking (Tube) approach that does not require a detailed velocity field.

Research Group

AbdelKarim Abulaban, Research Associate
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Debasmita Misra, Research Associate
Cam Nguyen, Research Associate
Hung Viet Nguyen, Graduate Student Researcher
Paul Oduro, Graduate Student Researcher

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Department of Horticulture

Mark Brenner

Mark Brenner, Principal Investigator

Structure and Activity Relationships of Plant Growth Substances

During the past several decades, there has been intensive work characterizing the response of various plant growth substances on plant growth and development. Surprisingly, understanding of the specific structural components that determine biological activity is not fully understood. These researchers are collaborating with several plant hormone scientists in several different countries to assemble some accurate structural models that account for the observed activity of these molecules. Initially, they will focus on the Auxin derivatives of Indole-3-Acetic Acid and some of the Gibberellins. The molecular weight range for the majority of plant hormones is 150ï¿½700 Daltons. A variety of available computer programs are currently being tested and explored to determine the most appropriate for follow up studies.

Research Group

Gerald L. Pierson, Nonacademic Staff

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Department of Soil, Water, and Climate

Kenneth J. Davis
Satish C. Gupta

Kenneth J. Davis, Principal Investigator

Modeling the Influence of Atmospheric Boundary Layer Processes on Biogenic Hydrocarbon Mixing and Chemistry

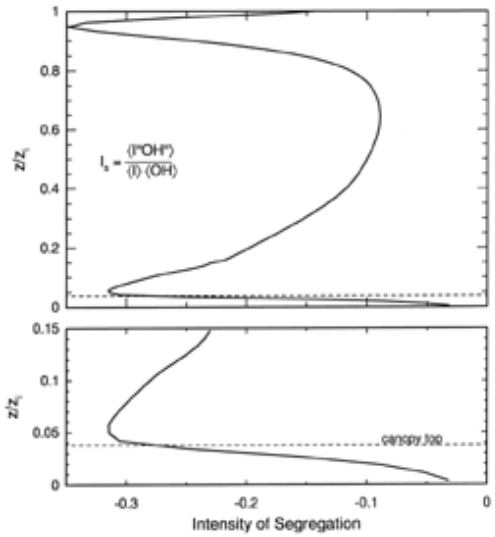
The primary objectives of this research are to study how lower atmospheric turbulence and cloud formation influence ozone-hydrocarbon photochemistry. These researchers plan to focus on how cumulus clouds, a forest canopy, spatial variations in forest hydrocarbon emissions, and chemical lifetimes influence the chemistry of the lower atmosphere.

These micro-scale processes are important in the formation of lower atmospheric ozone pollution. Ozone pollution is most often a problem during stagnant, sunny, summer conditions when cumulus clouds and lower atmospheric convective mixing are common. Ozone is produced by the interaction of hydrocarbons, nitrogen oxides, and sunlight. Trees emit large quantities of hydrocarbons and complicate lower atmospheric mixing by sequestering hydrocarbon-rich air within their canopy. Therefore, studying the lower atmosphere and cumulus clouds over forested regions is of great relevance to the ability to understand and predict ozone pollution events. Small-scale mixing of short-lived hydrocarbons and aqueous chemistry are likely to significantly impact ozone production. These effects have not been addressed to date. This is largely due to the need to merge substantial meteorological and chemical expertise along with extensive computing resources.

The model being used by these researchers to resolve turbulent motions within the convective boundary layer (CBL) is the National Center for Atmospheric Research large eddy simulation (LES) model. The model uses a wave-cutoff filter to define the resolvable-scale variables and parameterizes the subgrid-scale effects with a turbulence energy model. The LES model computes Navier-Stokes equations for three components of the resolvable-scale velocity, the conservation equation for potential temperature, the Poisson equation for the pressure field, and the subgrid-scale kinetic energy equation. Horizontal advection is calculated using the pseudospectral method and vertical advection is calculated using the centered finite-difference scheme. To advance in time, the code uses a third-order Runge-Kutta scheme.

The newest version of the LES, which allows for multiple regions of grid nesting, was combined with the dynamical effects of a forest canopy into the fine resolution region located at the surface. This nested model can resolve canopy scales of motion and examine their influence on the full CBL. This coupled forest canopy-CBL LES is being used to study the influence of the forest on biogenic hydrocarbon mixing in the CBL.

An updated version of the National Center for Atmospheric Research regional chemistry model provides the chemical mechanism. Because the set of chemical reactions presents a stiff set of differential equations, an approximate solution technique, the Euler Backward Iterative (EBI), is being used. This chemical mechanism, merged with the LES, is finally used to study the influence of micro-scale mixing in the cloud-free CBL on ozone photochemistry.



The turbulence-induced segregation between two chemical reactants in the convective boundary layer and a forest canopy from which the ï¿½Iï¿½ reactant is emitted. z is altitude above ground,

and zi is the convective boundary layer depth (about 1 kilometer). Brackets denote a horizontal domain average. Double-prime denotes fluctuations about this mean. OH is produced throughout the domain and reacts with isoprene (I). Results are from a nested convective boundary layer-forest canopy large eddy simulation.

Research Group

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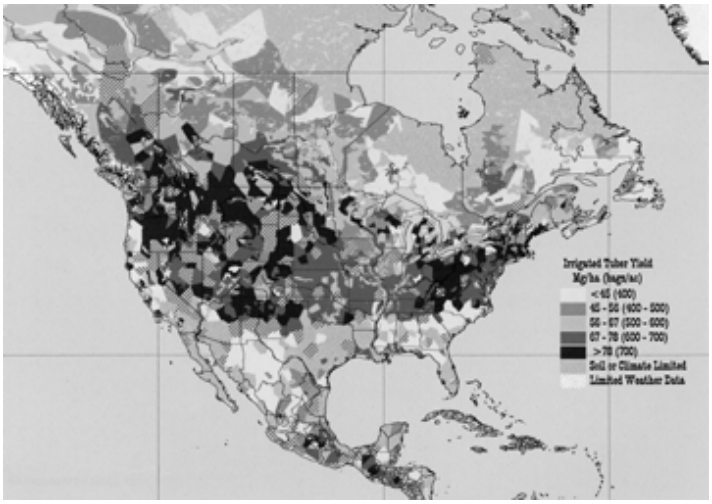
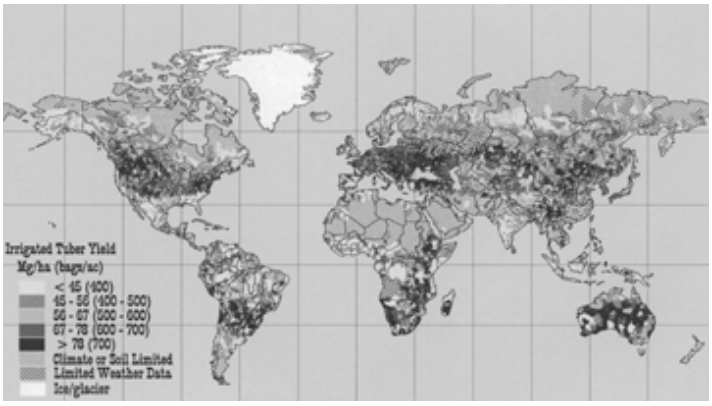
Satish C. Gupta, Associate Fellow

Delineating Potato Growing Areas Around the World

With expanding World markets, many of the fast food corporations are interested in opening franchises in remote parts of the World. One of the major food items served is french fries. In the United States, french fries are mostly made from the Russet Burbank potato. There is some interest in companies that supply french fries to the fast food corporations to identify areas around the World where Russet Burbank variety of potato can be grown effectively. This research delineated areas around the World where Russet Brubank variety can be grown without any major limitations. The procedure involved linking the World soil and climate databases to the SIMPOTATO computer model through the Geographic Information System (GIS). The World soil database consisted of 5,000 map units. Important soil factors included texture, slope, soil depth, pH, and organic carbon. The climate database contained maximum and minimum air temperatures, and precipitation from 1977 through 1991 for 10,000 stations around the Globe. It also included the latitude, longitude, and elevation of the weather station. Daily solar radiation was approximated from the maximum and minimum air temperatures and the solar constant. The two databases were overlaid each other to delineate 90,000 polygons for yield predictions. The model was run in increments of 500 polygons and the simulation results were stored into one file for each of the 10 World areas. Geographical Information System (GIS) was then used to produce potato yield maps of the World. In general, there were two high potato-yielding regions (35-55 iN latitude and 25- 40 iS latitude) around the Globe. The lack of symmetry in potato yield around the equator is most likely due to ocean mediating temperatures especially in the Southern Hemisphere. The United States and Europe showed the highest yield potential for irrigated Russet Burbank production. There were also regions along the border of Mongolia and China that showed potential for high potato yield. This work is being done in cooperation with Professor J.F. Moncrief, C.J. Rosen, and C.A. Thill of the Horticulture Science and Soil, Water, and Climate Departments at the University of Minnesota.



Simulation of Russet Burbank tuber irrigated yields for portions of the United States, Canada, and Mexico.



Irrigated tuber yield for the Russet Burbank variety around the World.

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Cell Growth Dynamics of Unicellular Organisms under Changing Environmental Conditions

Cell properties such as mass, protein content, DNA content, and others are typically distributed among the cells of a population due to the operation of the cell cycle. Furthermore, cell growth exhibits very different patterns during each stage of the cell cycle. A mathematical model has been developed that takes the distributed and staged nature of cell growth into account. The model consists of a system of population balance equations, each describing a different stage of the cell cycle, and an integro-ordinary differential equation accounting for substrate consumption. Using a time-explicit, finite difference scheme, the problem was solved for the case of a single variable and constant substrate concentration. A similar algorithm was used to solve the single-variable, single-staged model under conditions of changing substrate concentration. These researchers are currently working on the expansion of the numerical method in order to achieve the solution of the multi-staged, multi-variable cell population balance models in an environment of changing substrate concentration.

This project is solving multi-variable, multi-staged cell population balance models to predict time evolution of property distributions in cell populations of unicellular organisms such as Tetrahymena Pyriformis and Saccharomyces cerevisiae. Based on the relative content of DNA, the cell cycle is typically considered to consist of three distinct phasesï¿½the G1 phase where relative DNA content is one, the S phase where relative DNA content increases from one to two, and the G2 + M phase where relative DNA content remains two. Taking this structure of the cell cycle into account, growth dynamics during the exponential phase of a batch cell culture can be modeled.

Presently, these researchers have solved the problem formulated for the special case of a single variable (the physiological state vector consists of a single element) and for constant substrate concentration. The solution was achieved with the use of a time-explicit, one-step, finite difference scheme. Furthermore, using similar algorithms, a solution has been obtained for the single-staged, single-variable, mass structured cell population balance model under conditions of changing substrate concentration. Several simulations have been performed for different types of growth rate expression and equal and unequal partitioning; qualitative and quantitative differences between the cases of constant and changing substrate concentration have been studied. The researchers are now working on expanding existing numerical algorithms to higher dimensions. Both finite difference methods and various spectral methods are being considered.

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Victor Bloomfield
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Alex J. Lange
John D. Lipscomb
Rex Lovrien
Kevin Mayo
Douglas H. Ohlendorf
David D. Thomas

Norma M. Allewell, Principal Investigator

Structure Determination and Modeling of Electrostatic Effects in Large Macromolecules

These researchers have developed a rapid, self consistent method for calculating electrostatic potentials, pKa values, and titration curves based on the Multigrid Poisson-Boltzmann (MGPB) approach. The method has been applied to a large, multisubunit protein, E. coli aspartate transcarbamylase. Long range interactions have been identified in the unliganded crystal structure, and titration curves obtained with the MGPB method have been shown to agree well with experiment. These calculations have been carried out for the different states of the protein, ligated with the substrate N-phosphonacetyl-L-aspartate (PALA), inhibitor cytosine-5'-triphosphate (CTP), and both phosphonacetamide and malonate with CTP. Electrostatic modeling of additional ligated structures is helping to understand the changes in electrostatics due to ligation. Preliminary MGPB analysis has been performed on the crystal structures of wild type and mutant ferritins. The X-ray crystal structure of ornithine transcarbamylase (OTCase) in complex with its bisubstrate analog N-(phosphonacetyl)-L-ornithine (PALO) has been solved. The crystal structural determination of wild type human OTCase and several mutants are in progress. Modeling electrostatic effects in these structures give an understanding of their roles in driving conformational change, catalysis, and regulation.

Specific work is being done on ferritinsï¿½a family of proteins that can sequester large numbers of either ferrous or ferric iron in an organic phase inside the protein coat and concentrates. All ferritin molecules consist of a thin layer of the protein surrounding the polynuclear iron core. The assembled protein is stable with or without the iron core, which can be added or removed experimentally. Each ferritin comprises of a combination of L-, M-, and H-ferritins. L-ferritin differs from H- and M-ferritins in terms of rates of transport, oxidation, and nucleation of iron. Sequences of ferritin from higher organisms exhibit high homology. The three-dimensional structure of the bullfrog red cell L-ferritin has already been solved in the laboratory by these researchers. Structure determination of the H- and M-ferritin structures are currently in progress. Initial electrostatic calculations of L-ferritin has shown that electrostatic properties play an important role in its function. Calculations of the three classes of ferritins and a comparison should reveal an analogy between its electrostatic properties and differences in their function. An electrostatics package developed by this group that uses the multigrid method to solve the nonlinear Poisson-Boltzmann equation was installed and adapted for parallel computing.

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Ian Armitage, Principal Investigator

Nuclear Magnetic Resonance Methods for Macromolecules in Biological Processes

This research groupï¿½s activities revolve around the use of Nuclear Magnetic Resonance (NMR) methods to elucidate the solution tertiary structure of macromolecules involved in biological processes. Specifically, the group is looking at processes including proteins involved in cellular metal homeostasis, biomolecules involved in the immune response, and the DNA-binding domain (DBD) of the human vitamin D receptor (hVDR) and its complex with specific elements of DNA. The premise is that functional details are contained within a knowledge of the structure at atomic resolution. The computers at the Supercomputing Instituteï¿½s Basic Sciences Computing Laboratory and numerous software packages are being used in this work. Software packages VNMR and NmrPipe are being used for NMR processing, X-PLOR is being used for structure calculations, and Insight II, MOLMOL, MacroModel, and GRASP are being used for visualization and analysis of three-dimensional structures.

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Structure and Function Studies of Biological Macromolecules

X-ray structures of intracellular lipid binding proteins have been completed in this laboratory. The researchers are carrying out in depth structure/function studies via protein engineering so that the ligand specificity within this protein family is definable by a systematic set of chemical rules. One objective is to convert the fatty acid specificity of Adipogyte Lipid Binding Protein (ALBP) to a high affinity retinoic acid site, imitating the unique Cellular Retinoic Acid Binding Protein I (CRAPBI) retinoid specificity.

Research toward understanding the structure-function relationships present in Short Chain Hydroxyacyl Coenzyme A Dehydrogenase (SCHAD), a mitochondrial enzyme involved in the metabolism of fatty acids, is underway. Kinetic characterization, site-directed mutagenesis, and rational inhibitor design studies are planned to study the enzyme mechanism. Structural characterization of SCHAD provides information for molecular modeling of analogous proteins. This helps to explain functional deficiencies and associated disease states for SCHAD and its analogous proteins.

The X-ray structure of two lipoproteins were recently solved and are being refined. Microsomal transfer protein (MTP) is involved in lipid transport and is required for very low density lipoprotein assembly. The smaller subunit of MTP has been identified as protein disulfide isomerase. Although the in vivo roles of the two subunits are not yet clear, structural characterization may provide important clues. A domain of MTP has sequence similarity to that of a highly helical segment of lipovitellin (LV). An existing LV model is being refined with a new cryogenic X-ray data set that allows construction of previously disordered portions of LV and its bound lipid.

Building on structural information from prior X-ray analyses of E. coli and mitochondrial Malate Dehydrogenase (MDH), this group is studying MDH catalysis, biological function, and protein import. The groundwork has been achieved by the preparation of an MDH(-) strain of E. coli, several mutant forms of the E. coli MDH protein, and the crystallization and X-ray data collection of precursor forms of MDH. A three-dimensional structure of the pre-glyoxysomal MDH is underway.

The homotetrameric Phosphoglycerate Dehydrogenase (PGDH) catalyzes the first key committed step in the serine biosynthetic pathway. This groupï¿½s completed PGDH structure shows each subunit comprised of a substrate binding domain, a nucleotide binding domain, and a regulatory binding domain. The substrate and nucleotide binding domains resemble related dehydrogenases and potentially remove regulation by free serine. The structure of this truncated protein probe is being solved to find the importance of the conserved quaternary structure in function.

Many of the effects of 1,25-dihydroxyvitamin D3 in growth and development are mediated by Vitamin D Nuclear Receptor Protein (VDR), a transcription factor that is structurally related to other members of the steroid/thyroid superfamily of nuclear receptors. It is comprised of discrete DNA and ligand binding domains. The DNA binding domain has putative zinc finger regions believed to bind to unique DNA sequences in vitamin D responsive genes. The manner with which VDR binds to DNA is not known. It has been hypothesized that DNA binding by the zinc finger regions is triggered after conformational changes have been induced by the binding of 1,25-vitamin D3 to its ligand binding domain. This continued work is determining the X-ray crystal structure of the 1,25-vitamin D3 receptor and postulate plausible mechanisms of ligand induced DNA binding.

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Interacting DNA Systems

The regulation of gene expression is controlled by specific protein-DNA interactions that serve to activate or inhibit cellular protein biosynthesis. In vivo, these reactions take place in a milieu that is highly volume occupied (greater than thirty-five of the volume percentage) by nonreactive DNA and other macromolecules. The effect of this solution crowding and the accompanying strong intermolecular interactions on the kinetics of these interactions has become an important question in molecular biophysics.

These researchers have been working to develop a Brownian dynamics simulation technique for computing the time-dependent bimolecular rate constant for site-specific protein binding to DNA in the presence of non-reactive, background molecules (crowding agents). This code is used to explore the effect of strong excluded volume and electrostatic interactions on both diffusion and the rate of the reactions. Due to the large number of particles in the simulations and the long trajectories necessary to

achieve meaningful results, most of the efforts have been focused on developing more computationally efficient methods that remain realistic.

Past work focused on the effect of spherical crowding agents on these kinetics in both the presence and absence of electrostatic interactions between the reactive protein and DNA. This group was able to demonstrate that the reduction in reaction rate in the presence of increasing concentrations of background particles exactly paralleled the reduction in mobility of the reactive probe, and this result was independent of the nature and magnitude of the electrostatic interactions. While there is currently no relevant experimental data to which the results may be compared, this behavior is consistent with theoretical predictions for the effect of volume occupancy on reaction rates, and it is believed that this supports the validity of the simulation method.

Presently, these researchers are extending their simulations to include chains or rods as background particles. While they expect that this change in particle geometry will make little difference in the absence of electrostatic interactions, it has been suggested that attractive electrostatic interactions between a diffusing spherical particle (the protein) and rod-like polyelectrolytes could lead to enhanced sphere mobility due to alternate one-dimensional sliding and hopping along and between the rods. The researchers are working out simulations of the protein binding rate as a function of background chain (rod) concentration in both the presence and absence of electrostatic interactions. Data from these simulations are analyzed for evidence of sliding and hopping behavior by characterizing the concentration dependence of both the rate constant and the protein mobility.

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Bianca M. Conti-Fine, Principal Investigator

Molecular Modeling of Diphtheria Toxin

The purpose of modeling the diptheria toxin molecule is to generate diagrams of sequence regions and planking loops. This research has identified the sequence regions of diphtheria toxin recognized by CD 4+ T cells of healthy humans of different major histocompatibility complex haplotypes. These diagrams are generated by molecular modeling software. The packages use files obtained from the Brookhaven Protein Data Bank.

Research Group

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Alex J. Lange, Principal Investigator

Hormonal Control of Hepatic Gluconcogenesis/Glycolysis

The level of glucose in the blood is determined, at least in part, by the gluconeogenic/glycolytic status of the hepatic carbohydrate metabolic flux. A major player in the control of hepatic carbohydrate fluxes is fructose-2,6-bisphosphate. This small sugar phosphate elicits the switch from glycolytic to gluconeogenic (and vice versa) by allosterically activating 6-phospho- fructo-1-kinase and inhibiting fructose-1,6-bisphosphatase. The hepatic level of Fru-2,6-P2 is determined by the bifunctional enzyme 6-phosphofructo-2-kinase/fructose-2,6-biphosphatase that synthesizes and degrades F-2,6-P2 at discrete sites in the macro-molecule. The bisphosphatase domain can be expressed separately in an E. coli expression system, and the crystal structure has been determined. Nuclear magnetic resonance spectroscopic techniques are currently being used to determine the charge state of catalytic residues and to clarify the molecular mechanism of bisphosphatase. Such studies are important in the treatment of diabetes because inhibition of bisphosphatase could lower blood glucose levels.

Research Group

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John D. Lipscomb, Principal Investigator

Structure and Mechanism of Oxygenase Enzymes

Oxygenase enzymes utilize molecular oxygen to oxidize a wide range of biological and manmade compounds with the incorporation of one or both atoms of oxygen into the products.

One project this group is working on involves a series of dioxygenase enzymes. These enzymes attack aromatic substrates with two hydroxyl substituents. The products are ring open compounds containing both atoms of oxygen from O2. These products are easily degraded by bacteria, thus allowing the enormous amounts of carbon stored in aromatic compounds in the environment to reenter the carbon cycle. Also, the dioxygenases allow manmade aromatics, some of which are carcinogens, to be degraded. The crystal structures for three of these enzymes have already been solved.

Another class of oxygenase being studied is typified by methane monooxygenase. This enzyme catalyzes the oxidation of methane to methanol with the incorporation of one atom of oxygen. Methane is generated in large quantities in the environment and is a potent greenhouse gas. It is prevented from reaching the atmosphere by the action of methane monooxygenase. The crystal structure has been solved for the critical hydroxylase component and the supercomputing resources at the Institute are being used to visualize the structure and plan mutagenesis studies.

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Binding of Sulfonates to Proteins

These researchers use supercomputing resources to investigate the structures of sulfonates and related compounds. They make use of the Cambridge Crystallographic Database to search for solved sulfonate structures. These structures are then investigated, and possible protein-binding schemes are modeled. Structures of sulfonate cocrystals with oligopeptides are of particular interest. Investigation is also being done on sulfonate ligand binding to proteins using the database as a reference source of solved structures of low molecular weight. Structures with ion pairs are of special interest in this facet of the work.

Research Group

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Kevin Mayo, Principal Investigator

Structure and Dynamics of Proteins and Peptides

This laboratory is investigating the structure and dynamics of proteins and peptides using nuclear magnetic resonance (NMR) spectroscopy. Following derivation of inter-nuclear distance and angular constraints from various NMR experiments, computational modeling is performed in order to derive the best set of structures to the experimental data. Simulated annealing and molecular dynamics calculations are used in the protocol to derive the structure, and relaxation matrix calculations are used during structural refinement.

Relatedly, this laboratory is also interested in understanding internal motions in proteins and peptides. Molecular dynamics simulations are being used in conjunction with NMR relaxation experiments on isotopically enriched peptides and proteins to derive information on the motional frequencies and amplitudes of backbone and side-chain bond vectors.

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Structural Analysis of Macromolecules

The work in this laboratory involves creating and refining structural models of macromolecules using diffraction data, geometric constraints, and structures of homologous molecules. These researchers are producing sufficiently accurate models to gain insight into the structural foundations for their biological functions. The predictions made by these models are checked through biophysical analysis of complexes and mutants of targeted proteins.

Work on Protocatechuate 3,4-dioxygenase (PCD) involves PCDs from three organismsï¿½Pseudomonas putida, Brevibacterium fuscum, and Acinetobacter calcoaceticus. Dioxygenases carry out a unique reaction in which molecular oxygen is induced to cleave an aromatic ring. This reaction is important because it is used by bacteria to degrade a number of toxic compounds that contaminate the environment. This reaction is interesting because cleavage of a stable aromatic ring occurs without the use of exotic cofactors. In PCD, the cleavage is accomplished by a non-heme ferric ion in the active site.

Other work is being done on Homoprotocat-echuate 2,3-dioxygenase (HPCD). Like PCD, a single metal ion is used to cleave an aromatic ring. Unlike PCD, this cleavage is adjacent to the vicinal hydroxyls and utilizes a non-heme ferrous ion or a manganese ion. This group has crystallized HPCD from two organisms in two crystal forms and is working to solve their structures.

Like PCD, Catechol 1,2-dioxygenase (CTD) from Pseudomonas arvilla, incorporates both atoms of molecular oxygen into an organic substrate using a non-heme ferric ion. However, where the PCDs being studied contain six or more protomers, CTD contains only a single protomer. In addition, the substrate specificity is different in that CTD does not require the presence of a carboxylate group on the aromatic ring.

Further work is being done on toxic shcok syndrome toxin-1 (TSST-1). TSST-1 from Staphylococcus aureus is the causative agent in toxic shock syndrome and is a member of a family of pyrogenic toxins that have been referred to as superantigens. Typically, 0.0001%ï¿½0.01% of helper CD4+ T-cells respond when presented with an antigen. However, when a superantigen such as TSST-1 is present, as many as 20% of these helper T-cells respond by releasing large amounts of cytokines producing fever, vomiting, diarrhea, shock, and sometimes death. Through the production of mutants of TSST-1, this group hopes to be able to modulate these activities.

Exfoliative toxins A (ETA) and B (ETB) from Staphylococcus aureus are the last systems being studied. ETA toxin is the causative agent in staphylococcal scalded skin syndrome. Although it is a superantigen, there is no structural homology with other superantigens.

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Muscle Biomolecular Dynamics

The goal of this work is to understand the molecular motions that occur during muscle contraction and to correlate these motions to muscle biochemical and mechanical states. The researchers are using electron paramagnetic resonance (EPR) and time-resolved optical spectroscopy because they yield useful data from dynamic and disordered systems. By attaching reporter groups, either spin labels or luminescent dyes, to the proteins of interest, this group can examine them in solution and in situ. The group is applying their current routines to fit experimental data, simulate the structures and dynamics of their probes, and simulate spectra based on the molecular dynamics simulations.

The EPR spectrum of a spin-labeled protein is complex, formed from a continuum of spin label signals corresponding to differing orientation and motion. The researchers use several strategies to extract information about spin label orientation and motion from these spectra. The strategies all entail spectral simulation, either for direct use as reference spectra or indirect use in a fitting routine. As the group has begun to use global analysis, they found that the effective parameters no longer provide adequate fits to all spectra simultaneously, and therefore, they must explicitly model the effects of probe motion. They have written codes to solve systems of diffusion-coupled Bloch equations. They have also developed routines to simulate EPR spectra directly from a trajectory that gives the probeï¿½s orientation over time. These routines are particularly useful when combined with molecular dynamics simulations where there is no simple model describing the probeï¿½s motion.

Time-resolved optical data is recorded as decay in the absorption or emission anisotropy after the probe is excited by a pulse of polarized laser light. Analysis of this data has usually involved simulating exponential decays repeatedly. The group has also implemented diffusion-rate and analytical models of decays from molecular motion. They have been able to extend their analysis of the rotational dynamics of actin filaments beyond the simple analytical models to the Schurr torsional-twist model that takes all interprotomer interactions in the filament into account. The simulations are repeated for the subranges of the filament length, and the fitting routine uses the combined simulation. The group is continuing to use this approach to investigate the behavior of actin filaments with actin-binding proteins attached. The model of motion for the myosin head was wobble-in-a-band (WIB), a diffusion model borrowed from EPR simulations. Fitting is being performed using the WIB routines. Finally, routines to simulate anisotropy decays are being developed based on the molecular dynamics simulations.

The group has successfully used spin labels attached to the regulatory light chain of myosin to detect a change of angle in myosin during muscle contraction, but they have not been able to convert it to an orientation of the myosin molecule because they do not know the orientation of the spin label on the myosin head. Moreover, they have a number of candidate residues that can be engineered into cysteine residues in myosin light chains that must be evaluated for effectiveness before producing the mutant light chains. The simulation of motions of spin labels and optical probes are being investigated when attached to myosin. While myosin is too large for normal molecular dynamics simulations, it is possible to use molecular dynamics to model the motion of the probes when attached to a simplified myosin molecule.

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Structure Determination and Modeling of Electrostatic Effects in Large Macromolecules

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Ian Armitage, Principal Investigator

Nuclear Magnetic Resonance Methods for Macromolecules in Biological Processes

This research groupï¿½s activities revolve around the use of Nuclear Magnetic Resonance (NMR) methods to elucidate the solution tertiary structure of macromolecules involved in biological processes. Specifically, the group is looking at processes including proteins involved in cellular metal homeostasis, biomolecules involved in the immune response, and the DNA-binding domain (DBD) of the human vitamin D receptor (hVDR) and its complex with specific elements of DNA. The premise is that functional details are contained within a knowledge of the structure at atomic resolution. The computers at the Supercomputing Instituteï¿½s Basic Sciences Computing Laboratory and numerous software packages are being used in this work. Software packages VNMR and NmrPipe are being used for NMR processing, X-PLOR is being used for structure calculations, and Insight II, MOLMOL, MacroModel, and GRASP are being used for visualization and analysis of three-dimensional structures.

Research Group

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Leonard J. Banaszak, Associate Fellow

Structure and Function Studies of Biological Macromolecules

X-ray structures of intracellular lipid binding proteins have been completed in this laboratory. The

researchers are carrying out in depth structure/function studies via protein engineering so that the ligand specificity within this protein family is definable by a systematic set of chemical rules. One objective is to convert the fatty acid specificity of Adipogyte Lipid Binding Protein (ALBP) to a high affinity retinoic acid site, imitating the unique Cellular Retinoic Acid Binding Protein I (CRAPBI) retinoid specificity.

Research toward understanding the structure-function relationships present in Short Chain Hydroxyacyl Coenzyme A Dehydrogenase (SCHAD), a mitochondrial enzyme involved in the metabolism of fatty acids, is underway. Kinetic characterization, site-directed mutagenesis, and rational inhibitor design studies are planned to study the enzyme mechanism. Structural characterization of SCHAD provides information for molecular modeling of analogous proteins. This helps to explain functional deficiencies and associated disease states for SCHAD and its analogous proteins.

The X-ray structure of two lipoproteins were recently solved and are being refined. Microsomal transfer protein (MTP) is involved in lipid transport and is required for very low density lipoprotein assembly. The smaller subunit of MTP has been identified as protein disulfide isomerase. Although the in vivo roles of the two subunits are not yet clear, structural characterization may provide important clues. A domain of MTP has sequence similarity to that of a highly helical segment of lipovitellin (LV). An existing LV model is being refined with a new cryogenic X-ray data set that allows construction of previously disordered portions of LV and its bound lipid.

Building on structural information from prior X-ray analyses of E. coli and mitochondrial Malate Dehydrogenase (MDH), this group is studying MDH catalysis, biological function, and protein import. The groundwork has been achieved by the preparation of an MDH(-) strain of E. coli, several mutant forms of the E. coli MDH protein, and the crystallization and X-ray data collection of precursor forms of MDH. A three-dimensional structure of the pre-glyoxysomal MDH is underway.

The homotetrameric Phosphoglycerate Dehydrogenase (PGDH) catalyzes the first key committed step in the serine biosynthetic pathway. This groupï¿½s completed PGDH structure shows each subunit comprised of a substrate binding domain, a nucleotide binding domain, and a regulatory binding domain. The substrate and nucleotide binding domains resemble related dehydrogenases and potentially remove regulation by free serine. The structure of this truncated protein probe is being solved to find the importance of the conserved quaternary structure in function.

Many of the effects of 1,25-dihydroxyvitamin D3 in growth and development are mediated by Vitamin D Nuclear Receptor Protein (VDR), a transcription factor that is structurally related to other members of the steroid/thyroid superfamily of nuclear receptors. It is comprised of discrete DNA and ligand binding domains. The DNA binding domain has putative zinc finger regions believed to bind to unique DNA sequences in vitamin D responsive genes. The manner with which VDR binds to DNA is not known. It has been hypothesized that DNA binding by the zinc finger regions is triggered after conformational changes have been induced by the binding of 1,25-vitamin D3 to its ligand binding domain. This continued work is determining the X-ray crystal structure of the 1,25-vitamin D3 receptor and postulate plausible mechanisms of ligand induced DNA binding.

Research Group

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Victor Bloomfield, Principal Investigator

Interacting DNA Systems

The regulation of gene expression is controlled by specific protein-DNA interactions that serve to activate or inhibit cellular protein biosynthesis. In vivo, these reactions take place in a milieu that is highly volume occupied (greater than thirty-five of the volume percentage) by nonreactive DNA and other macromolecules. The effect of this solution crowding and the accompanying strong intermolecular interactions on the kinetics of these interactions has become an important question in molecular biophysics.

These researchers have been working to develop a Brownian dynamics simulation technique for computing the time-dependent bimolecular rate constant for site-specific protein binding to DNA in the presence of non-reactive, background molecules (crowding agents). This code is used to explore the effect of strong excluded volume and electrostatic interactions on both diffusion and the rate of the reactions. Due to the large number of particles in the simulations and the long trajectories necessary to achieve meaningful results, most of the efforts have been focused on developing more computationally efficient methods that remain realistic.

Past work focused on the effect of spherical crowding agents on these kinetics in both the presence and absence of electrostatic interactions between the reactive protein and DNA. This group was able to

demonstrate that the reduction in reaction rate in the presence of increasing concentrations of background particles exactly paralleled the reduction in mobility of the reactive probe, and this result was independent of the nature and magnitude of the electrostatic interactions. While there is currently no relevant experimental data to which the results may be compared, this behavior is consistent with theoretical predictions for the effect of volume occupancy on reaction rates, and it is believed that this supports the validity of the simulation method.

Presently, these researchers are extending their simulations to include chains or rods as background particles. While they expect that this change in particle geometry will make little difference in the absence of electrostatic interactions, it has been suggested that attractive electrostatic interactions between a diffusing spherical particle (the protein) and rod-like polyelectrolytes could lead to enhanced sphere mobility due to alternate one-dimensional sliding and hopping along and between the rods. The researchers are working out simulations of the protein binding rate as a function of background chain (rod) concentration in both the presence and absence of electrostatic interactions. Data from these simulations are analyzed for evidence of sliding and hopping behavior by characterizing the concentration dependence of both the rate constant and the protein mobility.

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Bianca M. Conti-Fine, Principal Investigator

Molecular Modeling of Diphtheria Toxin

The purpose of modeling the diptheria toxin molecule is to generate diagrams of sequence regions and planking loops. This research has identified the sequence regions of diphtheria toxin recognized by CD 4+ T cells of healthy humans of different major histocompatibility complex haplotypes. These diagrams are generated by molecular modeling software. The packages use files obtained from the Brookhaven Protein Data Bank.

Research Group

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Alex J. Lange, Principal Investigator

Hormonal Control of Hepatic Gluconcogenesis/Glycolysis

The level of glucose in the blood is determined, at least in part, by the gluconeogenic/glycolytic status

of the hepatic carbohydrate metabolic flux. A major player in the control of hepatic carbohydrate fluxes is fructose-2,6-bisphosphate. This small sugar phosphate elicits the switch from glycolytic to gluconeogenic (and vice versa) by allosterically activating 6-phospho- fructo-1-kinase and inhibiting fructose-1,6-bisphosphatase. The hepatic level of Fru-2,6-P2 is determined by the bifunctional enzyme 6-phosphofructo-2-kinase/fructose-2,6-biphosphatase that synthesizes and degrades F-2,6-P2 at discrete sites in the macro-molecule. The bisphosphatase domain can be expressed separately in an E. coli expression system, and the crystal structure has been determined. Nuclear magnetic resonance spectroscopic techniques are currently being used to determine the charge state of catalytic residues and to clarify the molecular mechanism of bisphosphatase. Such studies are important in the treatment of diabetes because inhibition of bisphosphatase could lower blood glucose levels.

Research Group

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John D. Lipscomb, Principal Investigator

Structure and Mechanism of Oxygenase Enzymes

Oxygenase enzymes utilize molecular oxygen to oxidize a wide range of biological and manmade compounds with the incorporation of one or both atoms of oxygen into the products.

One project this group is working on involves a series of dioxygenase enzymes. These enzymes attack aromatic substrates with two hydroxyl substituents. The products are ring open compounds containing both atoms of oxygen from O2. These products are easily degraded by bacteria, thus allowing the enormous amounts of carbon stored in aromatic compounds in the environment to reenter the carbon cycle. Also, the dioxygenases allow manmade aromatics, some of which are carcinogens, to be degraded. The crystal structures for three of these enzymes have already been solved.

Another class of oxygenase being studied is typified by methane monooxygenase. This enzyme catalyzes the oxidation of methane to methanol with the incorporation of one atom of oxygen. Methane is generated in large quantities in the environment and is a potent greenhouse gas. It is prevented from reaching the atmosphere by the action of methane monooxygenase. The crystal structure has been solved for the critical hydroxylase component and the supercomputing resources at the Institute are being used to visualize the structure and plan mutagenesis studies.

Research Group

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Rex Lovrien, Principal Investigator

Binding of Sulfonates to Proteins

These researchers use supercomputing resources to investigate the structures of sulfonates and related compounds. They make use of the Cambridge Crystallographic Database to search for solved sulfonate structures. These structures are then investigated, and possible protein-binding schemes are modeled. Structures of sulfonate cocrystals with oligopeptides are of particular interest. Investigation is also being done on sulfonate ligand binding to proteins using the database as a reference source of solved structures of low molecular weight. Structures with ion pairs are of special interest in this facet of the work.

Research Group

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Kevin Mayo, Principal Investigator

Structure and Dynamics of Proteins and Peptides

This laboratory is investigating the structure and dynamics of proteins and peptides using nuclear magnetic resonance (NMR) spectroscopy. Following derivation of inter-nuclear distance and angular constraints from various NMR experiments, computational modeling is performed in order to derive the best set of structures to the experimental data. Simulated annealing and molecular dynamics calculations are used in the protocol to derive the structure, and relaxation matrix calculations are used during structural refinement.

Relatedly, this laboratory is also interested in understanding internal motions in proteins and peptides. Molecular dynamics simulations are being used in conjunction with NMR relaxation experiments on isotopically enriched peptides and proteins to derive information on the motional frequencies and amplitudes of backbone and side-chain bond vectors.

Research Group

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Douglas H. Ohlendorf, Fellow

Structural Analysis of Macromolecules

The work in this laboratory involves creating and refining structural models of macromolecules using diffraction data, geometric constraints, and structures of homologous molecules. These researchers are producing sufficiently accurate models to gain insight into the structural foundations for their biological functions. The predictions made by these models are checked through biophysical analysis of complexes and mutants of targeted proteins.

Work on Protocatechuate 3,4-dioxygenase (PCD) involves PCDs from three organismsï¿½Pseudomonas putida, Brevibacterium fuscum, and Acinetobacter calcoaceticus. Dioxygenases carry out a unique reaction in which molecular oxygen is induced to cleave an aromatic ring. This reaction is important because it is used by bacteria to degrade a number of toxic compounds that contaminate the environment. This reaction is interesting because cleavage of a stable aromatic ring occurs without the use of exotic cofactors. In PCD, the cleavage is accomplished by a non-heme ferric ion in the active site.

Other work is being done on Homoprotocat-echuate 2,3-dioxygenase (HPCD). Like PCD, a single metal ion is used to cleave an aromatic ring. Unlike PCD, this cleavage is adjacent to the vicinal hydroxyls and utilizes a non-heme ferrous ion or a manganese ion. This group has crystallized HPCD from two organisms in two crystal forms and is working to solve their structures.

Like PCD, Catechol 1,2-dioxygenase (CTD) from Pseudomonas arvilla, incorporates both atoms of molecular oxygen into an organic substrate using a non-heme ferric ion. However, where the PCDs being studied contain six or more protomers, CTD contains only a single protomer. In addition, the substrate specificity is different in that CTD does not require the presence of a carboxylate group on the aromatic ring.

Further work is being done on toxic shcok syndrome toxin-1 (TSST-1). TSST-1 from Staphylococcus aureus is the causative agent in toxic shock syndrome and is a member of a family of pyrogenic toxins that have been referred to as superantigens. Typically, 0.0001%ï¿½0.01% of helper CD4+ T-cells respond when presented with an antigen. However, when a superantigen such as TSST-1 is present, as many as 20% of these helper T-cells respond by releasing large amounts of cytokines producing fever, vomiting, diarrhea, shock, and sometimes death. Through the production of mutants of TSST-1, this group hopes to be able to modulate these activities.

Exfoliative toxins A (ETA) and B (ETB) from Staphylococcus aureus are the last systems being studied. ETA toxin is the causative agent in staphylococcal scalded skin syndrome. Although it is a superantigen, there is no structural homology with other superantigens.

Research Group

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David D. Thomas, Fellow

Muscle Biomolecular Dynamics

The goal of this work is to understand the molecular motions that occur during muscle contraction and to correlate these motions to muscle biochemical and mechanical states. The researchers are using electron paramagnetic resonance (EPR) and time-resolved optical spectroscopy because they yield useful data from dynamic and disordered systems. By attaching reporter groups, either spin labels or luminescent dyes, to the proteins of interest, this group can examine them in solution and in situ. The group is applying their current routines to fit experimental data, simulate the structures and dynamics of their probes, and simulate spectra based on the molecular dynamics simulations.

The EPR spectrum of a spin-labeled protein is complex, formed from a continuum of spin label signals corresponding to differing orientation and motion. The researchers use several strategies to extract information about spin label orientation and motion from these spectra. The strategies all entail spectral simulation, either for direct use as reference spectra or indirect use in a fitting routine. As the group has begun to use global analysis, they found that the effective parameters no longer provide adequate fits to all spectra simultaneously, and therefore, they must explicitly model the effects of probe motion. They have written codes to solve systems of diffusion-coupled Bloch equations. They have also developed routines to simulate EPR spectra directly from a trajectory that gives the probeï¿½s orientation over time. These routines are particularly useful when combined with molecular dynamics simulations where there is no simple model describing the probeï¿½s motion.

Time-resolved optical data is recorded as decay in the absorption or emission anisotropy after the probe is excited by a pulse of polarized laser light. Analysis of this data has usually involved simulating exponential decays repeatedly. The group has also implemented diffusion-rate and analytical models of decays from molecular motion. They have been able to extend their analysis of the rotational dynamics of actin filaments beyond the simple analytical models to the Schurr torsional-twist model that takes all interprotomer interactions in the filament into account. The simulations are repeated for the subranges of the filament length, and the fitting routine uses the combined simulation. The group is continuing to use this approach to investigate the behavior of actin filaments with actin-binding proteins attached. The model of motion for the myosin head was wobble-in-a-band (WIB), a diffusion model borrowed from EPR simulations. Fitting is being performed using the WIB routines. Finally, routines to simulate anisotropy decays are being developed based on the molecular dynamics simulations.

The group has successfully used spin labels attached to the regulatory light chain of myosin to detect a change of angle in myosin during muscle contraction, but they have not been able to convert it to an orientation of the myosin molecule because they do not know the orientation of the spin label on the myosin head. Moreover, they have a number of candidate residues that can be engineered into cysteine residues in myosin light chains that must be evaluated for effectiveness before producing the mutant light chains. The simulation of motions of spin labels and optical probes are being investigated when attached to myosin. While myosin is too large for normal molecular dynamics simulations, it is possible

to use molecular dynamics to model the motion of the probes when attached to a simplified myosin molecule.

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College of Education

Lynne K. Edwards, Fellow

A Monte Carlo Study on Educational Statistics

This project contains both substantive goals as well as methodological goals. For the substantive interest, these researchers built a model for explaining psychological and sociological factors supporting the female students in mathematics and science courses. The methodological portion asked the question of effects of complex sampling designs and/or missing values on selected analytical procedures applied to the data with time-dependent structures. Solutions derived from the methodological segment will, in return, enhance the interpretability of the substantive questions from the large national database.

The methodological portion involves parameter estimation problems in dealing with missing values in time-dependent observations. There are several methods proposed to deal with missing data. Among the data imputation methods (as opposed to elimination of cases with missing values), the multiple imputation method is most promising. In principal component analysis, there has not been extensive research done with respect to the effects of missing values and the imputation (or deletion methods) in the derived components. Another concern is a hierarchical linear model hailed in modeling time-dependent observations with hierarchical structures. In addition, the appropriate degrees of freedom to be used in a complex sample design for the analytical methods chosen has not been explored. Often, the suggested estimators are derived from an iterative process. In order to suggest a reasonable robust approach to a data with time-dependent structure, there is a need to examine the effects of missing values, data imputation methods, effective degrees of freedom, and their impacts on a selected analytical procedure, namely, the hierarchical linear model. The time points are increasing every two years, thus more interesting questions on studentsï¿½ growth can be addressed.

A sizable storage and data manipulation memory is needed for this project using the national educational database, NELS. Because every two years, new followup data are added to the existing database, the size of the data matrix is ever increasing. Three subprojects being pursued require the use of highly iterative and nonlinear solutions for estimation and maximization of the missing data. These parameter estimations are then applied to selected analytical procedures. The third and fourth segments of the project involve numerical approximations to certain distributions. The iterative algorithm can be easily adapted to a high-performance parallel computer since the large matrices to be optimized have the structural parallelism as opposed to the data-parallelism.

Research Group

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Department of Economics

Gautam Gowrisankaran
Michael P. Keane
Marcel K. Richter

Gautam Gowrisankaran, Principal Investigator

Estimating Hospital Quality Using a Bayesian Selection Model

This project is estimating the quality of pneumonia care provided by hospitals in Southern California. These researchers posit an output-based approach where the main predictor of quality will be inpatient

mortality. A central problem with using mortality figures is selection bias. Good hospitals may attract sicker patients. Thus, hospital mortality figures will reflect both the quality of care and the severity of illness of the patients. The researchers attempt to control for unobserved patient severity of illness by using a Bayesian selection model. They model hospital choice as a function of geographical distance with a probit specification and then use the choice model to control for severity in the mortality equation. Thus, if a hospital is attracting patients from further distances, it may be because it is treating severely ill patients. This differential severity is reflected in the estimation of hospital quality. The use of Bayesian methods has a number of advantages. First, it allows the group to yield more precise results. Second, it allows them to test different, non-nested models of hospital quality easily.

Preliminary results indicate that, after controlling for selection, non-public, teaching hospitals have significantly better quality than average, while public hospitals have significantly worse quality than average. Moreover, standard probit estimation (without controls for unobserved selection) shows that these types of hospitals are not significantly different from the average hospital. This underscores the importance of controlling for unobserved patient selection.

Research Group

John Geweke, Faculty

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Michael P. Keane, Associate Fellow

Estimation of Discrete Stochastic Dynamic Programming Models of Economic Behavior using Monte-Carlo Integration

The substantive goal of this project is estimating dynamic models of how individuals make educational and occupational choices over the life cycle. It is necessary to model career choices in a dynamic context because current schooling and employment decisions result not only in current period rewards but lead to human capital accumulation that alters future wages. In such a situation, it is reasonable to model individuals as if they solve a discrete stochastic dynamic programming (DS-DP) problem in order to make optimal current period decisions.

Although most economists would agree that a DS-DP problem is the proper way to model choice behavior in such dynamic environments, implementation of such models has been severely limited by the computational burdens involved. Estimation of DS-DP models is computationally burdensome because it requires solving for the value functions at each point in the state space of the problem. These value functions are multiple integrals over the stochastic processes that drive decisions. As the number of choices grows, the number of state space points typically grows rapidly making it infeasible to evaluate all the necessary multiple integrals using numerical methods like quadrature.

These researchers have been working on Monte-Carlo methods to simulate the value functions in DS-DP problems and on interpolation methods in which the value functions at a subset of the state points is simulated and interpolated to the remaining state points. It appears that approximation errors in solution of DS-DP problems by such methods are small if care is taken in the choice of simulation and interpolation techniques. Use of such approximation methods makes it possible to estimate DS-DP

models with larger choice sets and more realistic state space representations than in previous work.

This project is using these new estimation methods to estimate dynamic models of educational and occupational choices over the life cycle. An estimated dynamic model of career choices can aid in the design of public policies such as tuition subsidies, unemployment insurance, and retraining programs for displaced workers. To give a specific example, this occupational choice model contains various occupations with different educational requirements as options. Recently, some economists have proposed the introduction of wage subsidies for low wage workers. Using the model, the effect of such subsidies has been simulated, and the findings show they would reduce the school attendance of young men. This is because the subsidies raise wages primarily in occupations that require little education making such occupations more attractive.

Recently, work was begun on a new model of educational and occupational choices of young women. This is a major extension of the basic model used for young men because it brings fertility and marriage in as additional decisions. Once completed, it will become possible to use this model to address a number of important questions about how public welfare policies aimed at women and children effect behavior.

This research is aiming to provide evidence on the practical usefulness of the simulation approach for estimation of DS-DP models. If the approach proves useful, it can lead to increased interestï¿½on the part of economistsï¿½in the use of supercomputers to estimate dynamic discrete choice models.

Michael P. Keane, Assoicate Fellow and Antonio Merlo, Co-Principal Investigator

A Political Economy Model of Congressional Careers

A fundamental question in political economy is why people decide to run for elections. Put differently, what are the returns to an individual from a career in politics? This project is looking to provide at least a partial answer to these fundamental questions and quantify the returns to a career in the United States Congress. To achieve this goal, these researchers are specifying a dynamic model of career decisions of a member of Congress and estimating this model using a new data set currently being collected.

Existing empirical studies of Congressional careers suffer from two limitations. They estimate static models in which politicians decisions about whether to run for the House of Representatives or for higher office depend only on current and not future rewards. They also ignore the possi- bility that representatives may decide to leave Congress to pursue alternative professional careers. This research overcomes both these limitations and provides a new framework for the empirical analysis of Congressional careers.

In this model, a politician first decides whether or not to run for the House of Representatives. If the person is elected, the next period carries the decision to run for re-election, run for election to higher office, exit politics for a private sector job, or retire from politics. If the politician decides to run for re-election or higher office, they face probabilities of winning in the elections. In order to choose among these options, the politician compares the expected payoffs associated with the different alternatives. If re-elected, the politician faces another set of choices in the next period.

The problem that politicians face is dynamic in the sense that the payoffs from each of the choice

options is not reflected only in current period rewards but also in future rewards. The payoff to winning a seat in Congress is not only the wage and prestige that a person receives from being in Congress for one term but also the increment in expected future payoffs that accrue as a result of election. In such a situation, it is reasonable to model individuals as if they solve a discrete stochastic dynamic programming problem in order to make optimal current period decisions.

A key feature in this model is that the potential career opportunities of politicians outside Congress is explicitly modeled. These researchers assure that when a politician exits from Congress, they can choose among a set of occupations, and the wage the politician would receive in each of these options is a function of the politicianï¿½s age, education, and congressional experience (i.e., number of terms in the House of Representatives, number of terms in the Senate, and committee assignments). Thus, the framework also sorts out the relative importance of two key factors that may induce people to pursue a political careerï¿½the utility politicians derive from being in Congress and the salaries they receive while in Congress versus the private sector returns to Congressional experience.

Finally, these researchers are using their estimated model to evaluate the effects of various interesting policy experiments on the value of a Congressional seat and on the career decisions of politicians. Such policies include the introduction of term limits, changes in the pension regime, changes in the wages in Congress, changes in the seniority rule for committee appointments, and so on.

Research Group

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Marcel K. Richter, Principal Investigator

Mathematical Economics

This researcher is investigating decision criteria for evaluation of efficiency in mathematical economics through high-performance computing.

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Department of Geography

Katherine Klink

Katherine Klink, Associate Fellow

Spatial and Temporal Land Surface Climatology

This project has two main foci. The first is spatial and temporal characteristics of the United States surface wind field. Access to high-quality climatological data series has become increasingly important in many areas of environmental research. Although wind is an important feature of surface climate and is routinely reported by weather observers, little effort has been devoted to compiling a data set that describes the temporal and spatial characteristics of surface winds. In this project, the researchers are using thirty years of hourly and three-hourly surface wind speed and direction observations at over two-hundred stations in the coterminous United States to derive a United States surface wind climatology. The climatological mean and variance of wind speed, direction, and velocity (wind vector) are examined along with temporal analyses of trends over the thirty year period. The objectives of this work are to complement existing temperature and precipitation climatologies by compiling a representative climatology of terrestrial surface winds within the United States and to examine the time series to determine if there exists any temporal trends in wind characteristics.

The second part of the project focuses on the modeling of regional climate and vegetation interactions in the Upper Great Lakes region of the United States (Minnesota, Wisconsin, and Michigan). Climate and vegetation in the Upper Great Lakes region have been influenced by continental-scale movement of air masses as well as by substrate types and regional features such as the Great Lakes and the prairie-forest border. For a better understanding of Holocene climate-vegetation interactions in the Upper Great Lakes region, regional models of climate (RegCM2) and flora/vegetation (STASH3 and FORSKA3) are used to evaluate land surface-atmosphere interactions for the present day and for eleven thousand, six thousand, and three thousand years ago. Output from these models are then linked to a pollen dispersion model (POLLSCAPE), and results are compared to observed fossil pollen from a high-quality, well dated regional pollen database. The similarity of predicted and observed pollen assemblages are used to evaluate climate predictions. When disagreements occur, their patterns in space and time are used to help identify sources of error. Sensitivity studies are used last to evaluate the modeling strategies.

Research Group

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Department of Wood and Paper Sciences

Timothy D. Larson
Shri Ramaswamy

Timothy D. Larson, Principal Investigator

Transverse Stiffener Beams in Timberdecks

This project uses a finite element code to simulate the structural behavior of a nail laminated timber bridge deck. The deck is analyzed as a system of solid planks, nail connectors, and stiffener beams. Design parameters for the stiffener beams are changed to study their impact on load sharing attributes of the deck system.

Research Group

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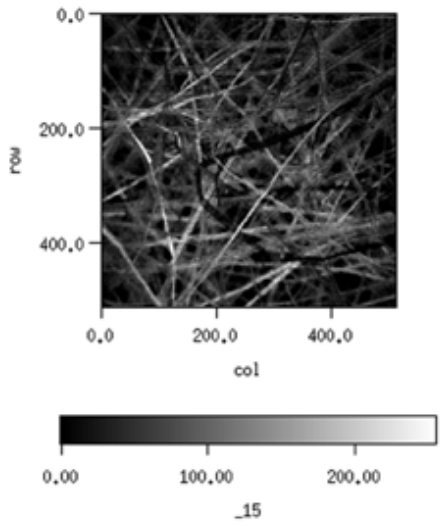
Shri Ramaswamy, Principal Investigator

Visualization and Characterization of Three-Dimensional Bulk Structure of Porous Materials

Structure of porous materials plays an important role both in the industrial manufacturing process and in many end-use applications. Flow or penetration of liquids in paper and paper board is very important in end-use applications such as writing, printing, and liquid packaging board (milk and juice cartons). In all cases, in addition to surface energy characteristics of the fibers, three-dimensional bulk structure of the porous material plays a critical role in the penetration of liquids. Until now, paper structures have been extremely simplified to consist of uniform cylindrical capillaries in explaining flow phenomena. This is primarily due to lack of better understanding of the structure and lack of sophisticated experimental techniques.

This research is visualizing and characterizing three-dimensional structures of paper using laser scanning confocal microscopy (LSCM). LSCM offers the ability to slice thin optical sections out of thick specimens and render an impressive three-dimensional, high-resolution view of biological specimens. Researchers have successfully used the LSCM technique to image the pore structure of geomaterials. However, they have not attempted to numerically characterize the pore structure. Using a fluorescent dye, the researchers were able to visualize cellulosic fiber materials and measure the fiber dimensions such as cell wall thickness, perimeter, and cross sectional area using an image analyzer. Here again, no attempt was made to evaluate the three-dimensional bulk structure of paper.

The researchers on this project are first visualizing the three-dimensional structure of paper using epi-fluorescent LSCM. The LSCM used for this purpose is a molecular dynamics laser scanning system. Scans of samples are being collected, visualized, and processed on an Indigo workstation. Further visualization and numerical deconvolution is being done to sharpen the image, minimizing the interference from multiple planes. Considering the amount of data from multiple planes even from one paper sample, parallel processing is imminent for numerical deconvolution. After this initial phase, if successful, numerical characterization of the three-dimensional surface will be investigated.



Confocal microscopy image of paper.

Research Group

Amit Goel, Graduate Student Researcher
Shuiyuan Huang, Research Associate

College of Liberal Arts

Department of Educational Psychology

Lynne K. Edwards

Lynne K. Edwards, Fellow

A Monte Carlo Study on Educational Statistics

This project contains both substantive goals as well as methodological goals. For the substantive interest, these researchers built a model for explaining psychological and sociological factors supporting the female students in mathematics and science courses. The methodological portion asked the question of effects of complex sampling designs and/or missing values on selected analytical procedures applied to the data with time-dependent structures. Solutions derived from the methodological segment will, in return, enhance the interpretability of the substantive questions from the large national database.

The methodological portion involves parameter estimation problems in dealing with missing values in time-dependent observations. There are several methods proposed to deal with missing data. Among the data imputation methods (as opposed to elimination of cases with missing values), the multiple imputation method is most promising. In principal component analysis, there has not been extensive

research done with respect to the effects of missing values and the imputation (or deletion methods) in the derived components. Another concern is a hierarchical linear model hailed in modeling time-dependent observations with hierarchical structures. In addition, the appropriate degrees of freedom to be used in a complex sample design for the analytical methods chosen has not been explored. Often, the suggested estimators are derived from an iterative process. In order to suggest a reasonable robust approach to a data with time-dependent structure, there is a need to examine the effects of missing values, data imputation methods, effective degrees of freedom, and their impacts on a selected analytical procedure, namely, the hierarchical linear model. The time points are increasing every two years, thus more interesting questions on studentsï¿½ growth can be addressed.

A sizable storage and data manipulation memory is needed for this project using the national educational database, NELS. Because every two years, new followup data are added to the existing database, the size of the data matrix is ever increasing. Three subprojects being pursued require the use of highly iterative and nonlinear solutions for estimation and maximization of the missing data. These parameter estimations are then applied to selected analytical procedures. The third and fourth segments of the project involve numerical approximations to certain distributions. The iterative algorithm can be easily adapted to a high-performance parallel computer since the large matrices to be optimized have the structural parallelism as opposed to the data-parallelism.

Research Group

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Qi Zhang, Graduate Student Researcher

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Department of Economics

Gautam Gowrisankaran
Michael P. Keane
Marcel K. Richter

Gautam Gowrisankaran, Principal Investigator

Estimating Hospital Quality Using a Bayesian Selection Model

This project is estimating the quality of pneumonia care provided by hospitals in Southern California. These researchers posit an output-based approach where the main predictor of quality will be inpatient mortality. A central problem with using mortality figures is selection bias. Good hospitals may attract sicker patients. Thus, hospital mortality figures will reflect both the quality of care and the severity of illness of the patients. The researchers attempt to control for unobserved patient severity of illness by using a Bayesian selection model. They model hospital choice as a function of geographical distance with a probit specification and then use the choice model to control for severity in the mortality

equation. Thus, if a hospital is attracting patients from further distances, it may be because it is treating severely ill patients. This differential severity is reflected in the estimation of hospital quality. The use of Bayesian methods has a number of advantages. First, it allows the group to yield more precise results. Second, it allows them to test different, non-nested models of hospital quality easily.

Preliminary results indicate that, after controlling for selection, non-public, teaching hospitals have significantly better quality than average, while public hospitals have significantly worse quality than average. Moreover, standard probit estimation (without controls for unobserved selection) shows that these types of hospitals are not significantly different from the average hospital. This underscores the importance of controlling for unobserved patient selection.

Research Group

John Geweke, Faculty

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Michael P. Keane, Associate Fellow

Estimation of Discrete Stochastic Dynamic Programming Models of Economic Behavior using Monte-Carlo Integration

The substantive goal of this project is estimating dynamic models of how individuals make educational and occupational choices over the life cycle. It is necessary to model career choices in a dynamic context because current schooling and employment decisions result not only in current period rewards but lead to human capital accumulation that alters future wages. In such a situation, it is reasonable to model individuals as if they solve a discrete stochastic dynamic programming (DS-DP) problem in order to make optimal current period decisions.

Although most economists would agree that a DS-DP problem is the proper way to model choice behavior in such dynamic environments, implementation of such models has been severely limited by the computational burdens involved. Estimation of DS-DP models is computationally burdensome because it requires solving for the value functions at each point in the state space of the problem. These value functions are multiple integrals over the stochastic processes that drive decisions. As the number of choices grows, the number of state space points typically grows rapidly making it infeasible to evaluate all the necessary multiple integrals using numerical methods like quadrature.

These researchers have been working on Monte-Carlo methods to simulate the value functions in DS-DP problems and on interpolation methods in which the value functions at a subset of the state points is simulated and interpolated to the remaining state points. It appears that approximation errors in solution of DS-DP problems by such methods are small if care is taken in the choice of simulation and interpolation techniques. Use of such approximation methods makes it possible to estimate DS-DP models with larger choice sets and more realistic state space representations than in previous work.

This project is using these new estimation methods to estimate dynamic models of educational and occupational choices over the life cycle. An estimated dynamic model of career choices can aid in the design of public policies such as tuition subsidies, unemployment insurance, and retraining programs

for displaced workers. To give a specific example, this occupational choice model contains various occupations with different educational requirements as options. Recently, some economists have proposed the introduction of wage subsidies for low wage workers. Using the model, the effect of such subsidies has been simulated, and the findings show they would reduce the school attendance of young men. This is because the subsidies raise wages primarily in occupations that require little education making such occupations more attractive.

Recently, work was begun on a new model of educational and occupational choices of young women. This is a major extension of the basic model used for young men because it brings fertility and marriage in as additional decisions. Once completed, it will become possible to use this model to address a number of important questions about how public welfare policies aimed at women and children effect behavior.

This research is aiming to provide evidence on the practical usefulness of the simulation approach for estimation of DS-DP models. If the approach proves useful, it can lead to increased interestï¿½on the part of economistsï¿½in the use of supercomputers to estimate dynamic discrete choice models.

Michael P. Keane, Assoicate Fellow and Antonio Merlo, Co-Principal Investigator

A Political Economy Model of Congressional Careers

A fundamental question in political economy is why people decide to run for elections. Put differently, what are the returns to an individual from a career in politics? This project is looking to provide at least a partial answer to these fundamental questions and quantify the returns to a career in the United States Congress. To achieve this goal, these researchers are specifying a dynamic model of career decisions of a member of Congress and estimating this model using a new data set currently being collected.

Existing empirical studies of Congressional careers suffer from two limitations. They estimate static models in which politicians decisions about whether to run for the House of Representatives or for higher office depend only on current and not future rewards. They also ignore the possi- bility that representatives may decide to leave Congress to pursue alternative professional careers. This research overcomes both these limitations and provides a new framework for the empirical analysis of Congressional careers.

In this model, a politician first decides whether or not to run for the House of Representatives. If the person is elected, the next period carries the decision to run for re-election, run for election to higher office, exit politics for a private sector job, or retire from politics. If the politician decides to run for re-election or higher office, they face probabilities of winning in the elections. In order to choose among these options, the politician compares the expected payoffs associated with the different alternatives. If re-elected, the politician faces another set of choices in the next period.

The problem that politicians face is dynamic in the sense that the payoffs from each of the choice options is not reflected only in current period rewards but also in future rewards. The payoff to winning a seat in Congress is not only the wage and prestige that a person receives from being in Congress for one term but also the increment in expected future payoffs that accrue as a result of election. In such a situation, it is reasonable to model individuals as if they solve a discrete stochastic dynamic programming problem in order to make optimal current period decisions.

A key feature in this model is that the potential career opportunities of politicians outside Congress is explicitly modeled. These researchers assure that when a politician exits from Congress, they can choose among a set of occupations, and the wage the politician would receive in each of these options is a function of the politicianï¿½s age, education, and congressional experience (i.e., number of terms in the House of Representatives, number of terms in the Senate, and committee assignments). Thus, the framework also sorts out the relative importance of two key factors that may induce people to pursue a political careerï¿½the utility politicians derive from being in Congress and the salaries they receive while in Congress versus the private sector returns to Congressional experience.

Finally, these researchers are using their estimated model to evaluate the effects of various interesting policy experiments on the value of a Congressional seat and on the career decisions of politicians. Such policies include the introduction of term limits, changes in the pension regime, changes in the wages in Congress, changes in the seniority rule for committee appointments, and so on.

Research Group

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Marcel K. Richter, Principal Investigator

Mathematical Economics

This researcher is investigating decision criteria for evaluation of efficiency in mathematical economics through high-performance computing.

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Department of Geography

Katherine Klink

Katherine Klink, Associate Fellow

Spatial and Temporal Land Surface Climatology

This project has two main foci. The first is spatial and temporal characteristics of the United States surface wind field. Access to high-quality climatological data series has become increasingly important in many areas of environmental research. Although wind is an important feature of surface climate and

is routinely reported by weather observers, little effort has been devoted to compiling a data set that describes the temporal and spatial characteristics of surface winds. In this project, the researchers are using thirty years of hourly and three-hourly surface wind speed and direction observations at over two-hundred stations in the coterminous United States to derive a United States surface wind climatology. The climatological mean and variance of wind speed, direction, and velocity (wind vector) are examined along with temporal analyses of trends over the thirty year period. The objectives of this work are to complement existing temperature and precipitation climatologies by compiling a representative climatology of terrestrial surface winds within the United States and to examine the time series to determine if there exists any temporal trends in wind characteristics.

The second part of the project focuses on the modeling of regional climate and vegetation interactions in the Upper Great Lakes region of the United States (Minnesota, Wisconsin, and Michigan). Climate and vegetation in the Upper Great Lakes region have been influenced by continental-scale movement of air masses as well as by substrate types and regional features such as the Great Lakes and the prairie-forest border. For a better understanding of Holocene climate-vegetation interactions in the Upper Great Lakes region, regional models of climate (RegCM2) and flora/vegetation (STASH3 and FORSKA3) are used to evaluate land surface-atmosphere interactions for the present day and for eleven thousand, six thousand, and three thousand years ago. Output from these models are then linked to a pollen dispersion model (POLLSCAPE), and results are compared to observed fossil pollen from a high-quality, well dated regional pollen database. The similarity of predicted and observed pollen assemblages are used to evaluate climate predictions. When disagreements occur, their patterns in space and time are used to help identify sources of error. Sensitivity studies are used last to evaluate the modeling strategies.

Research Group

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Kevin J. Lawless, Graduate Student Researcher

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Department of Wood and Paper Sciences

Timothy D. Larson
Shri Ramaswamy

Timothy D. Larson, Principal Investigator

Transverse Stiffener Beams in Timberdecks

This project uses a finite element code to simulate the structural behavior of a nail laminated timber bridge deck. The deck is analyzed as a system of solid planks, nail connectors, and stiffener beams. Design parameters for the stiffener beams are changed to study their impact on load sharing attributes of the deck system.

Research Group

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Shri Ramaswamy, Faculty

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Shri Ramaswamy, Principal Investigator

Visualization and Characterization of Three-Dimensional Bulk Structure of Porous Materials

Structure of porous materials plays an important role both in the industrial manufacturing process and in many end-use applications. Flow or penetration of liquids in paper and paper board is very important in end-use applications such as writing, printing, and liquid packaging board (milk and juice cartons). In all cases, in addition to surface energy characteristics of the fibers, three-dimensional bulk structure of the porous material plays a critical role in the penetration of liquids. Until now, paper structures have been extremely simplified to consist of uniform cylindrical capillaries in explaining flow phenomena. This is primarily due to lack of better understanding of the structure and lack of sophisticated experimental techniques.

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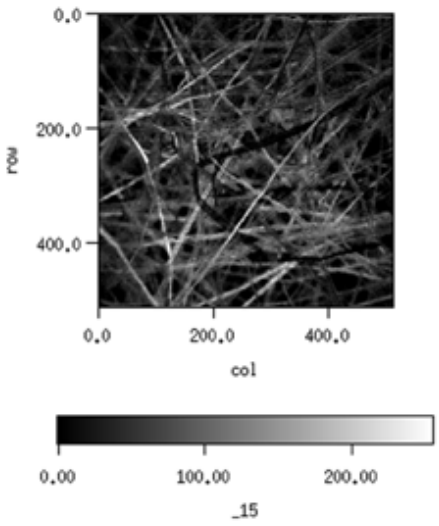


Confocal microscopy image of paper.

Research Group

Amit Goel, Graduate Student Researcher
Shuiyuan Huang, Research Associate

College of Pharmacy

David M. Ferguson, Fellow

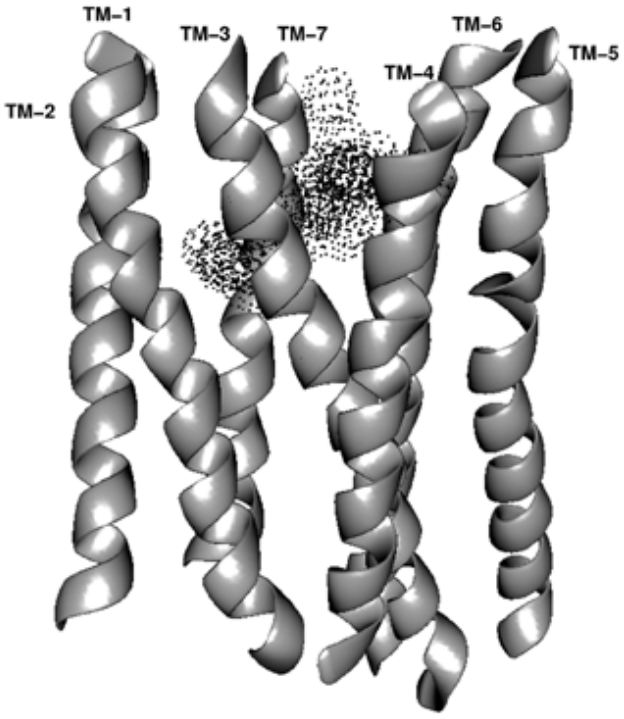
Computer Modeling of Biomolecular Processes and Ligand Recognition

This group has been active in several areas of applied supercomputing in an effort to study dynamic and thermodynamic properties of macromolecular structures and complexes. This work uses classical mechanical descriptions of molecular structures and interactions to simulate and explore the energy landscape of macromolecules using molecular dynamics and Monte Carlo methods. Projects range from statistical mechanical calculations of simple solutes in water to the prediction and de novo design of protein structures from first principles. Most projects involve development and implementation of new algorithms and methods for simulating molecular systems. This includes force field parameterization, development of simulation and analysis tools, and implementation of molecular dynamics and Monte Carlo codes on various supercomputing platforms.

Although a great deal of effort is devoted to the basic science of molecular modeling, this group focuses their efforts on solving highly applied problems in biocomputing. Currently, two major projects are underway. The first involves G protein-coupled receptors (GPCRs). GPCRs are the primary signaling mechanism on the cell surface and are involved in a wide variety of biological processes. Interest lies in the opioid family of GPCRs. These are responsible for antinociception or pain relief. Opiates have one great drawback, they are highly addictive. One goal of this work is to understand the structural basis for opiate binding at the opioid receptors in hope of designing less addictive drugs for

treating patients with chronic pain. However, this study is greatly complicated by the lack of a high-resolution model for the opioid GPCR. While they have many ligands that bind the opioid receptors, they have little evidence explaining why and where. This is the main goal of the work. To date, these researchers have built a model and defined the binding pockets for several opioid ligands. They have also provided some of the first glimpses as to why and where some opioid ligands bind. The current goal is to understand the selectivity displayed by certain ligand families. It turns out there are three opioid receptor types--m, d, and k--which elicit different pharmacological responses.

The second major focus of the work involves the development of antisense nucleic acids for use in gene therapy. Antisense therapies target messenger RNA (mRNA). The goal is to design a complimentary strand to tie up the messenger before it is translated to protein. In theory, if the protein causing disease is known, it should be able to be knocked out using antisense. However, the problem arises in the design of the antisense strand. These molecules must not only bind tightly to the target mRNA, but must be nuclease resistant (resistant to enzymes that degrade DNA in the body). This work focuses on understanding structural properties of synthetically modified nucleic acids to shed insight on the design of novel antisense molecules that are both tight binding and nuclease resistant. Work has recently been completed on the structural effect a 2'-sugar modification has on nucleic acid structure and stability. Investigations of a series of 2'-sugar substitutions is currently being investigated along with dynamic properties of single strand DNA.



Structural model of the dappa-opioid receptor with the putative ligand binding site filled with a sphere cluster for docking studies.

Research Group

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Divi Venkateswarlu, Research Associate

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David J.W. Grant, Principal Investigator

Crystal Structures and Molecular Simulations

Sulfonamides comprise a class of widely used antibacterial drugs. The crystal structures of various polymorphic phases have been solved and published. However, little work has focused on their solvates. In this laboratory, four sulfonamides (sulfapyridine, sulfadiazine, sulfamerazine, and sulfamethazine) were examined, and over a dozen solvates were discovered. The structures of these solvates are now being determined. The objectives of this study are to probe the intermolecular interactions between the drug and solvent in each solvate and to compare the crystal structures of the solvates with those of the parent drugs and among the solvates themselves. Ultimately, this group is gaining an understanding of how the solvent affects the properties of the drug and the reason behind the formation of each solvate. The researchers are working to predict solvate formation based on the structure of the drug.

Other work has been dealing with the prediction of tableting behavior from the crystal structures. From knowledge of the crystal structure of a pharmaceutical solid, obtained from the Cambridge Structural Database, the crystal properties are deduced. These properties are related to the mechanical properties of the material relevant to its ability to form tablets under compression, termed tableting performance. Hence, the overall focus of this work is on predicting the tableting performance of pharmaceutical materials from their crystal structure.

Research Group

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Deborah Kallick, Principal Investigator

Molecular Simulations of Biomolecules

Research in this laboratory uses data derived from nuclear magnetic resonance (NMR) spectroscopy to supplement holonomic constraints in restrained molecular dynamic simulations of RNA and other biological macromolecules. The majority of NMR spectroscopy laboratories determining structures of biological macromolecules in solution use approximations to the force field that lead to errors, especially in the treatment of electrostatic interactions. Typically, the NMR spectroscopy laboratory simulates the molecule in vacuo and simply turns off electrostatics.

A more realistic approach is to use the particle mesh Ewald method as implemented in AMBER, which has been computationally shown to result in stable simulations for large nucleic acids. The implementation of this method with the experimental restraints determined from solution NMR is one of the first of its kind on an RNA molecule. The goal of the work is to generate more realistic structures of macromolecules using both experimental data and computational techniques.

Other work involves analysis of NMR data and correlation of chemical shifts with structure. This work was begun in collaboration with Professor David Levitt of the Physiology Department at the University of Minnesota and was part of the Supercomputing Instituteï¿½s Undergraduate Internship Program last summer.

Research Group

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Daniel M. Kroll, Principal Investigator

Lattice Boltzmann Methods

Hydrodynamic interactions play a central role in determining dynamical and nonequilibrium phenomena in self-assembling amphiphilic systems and molecular aggregates in flow. In self-assembling fluids, correlated mesoscopic structures exist even far from criticality. It has been shown that this structure leads to anomalous scaling behavior in the dynamic structure factor as well as anomalies in the shear viscosity and attenuation and dispersion of sound. In flow, the deformation of these correlated domains gives rise to excess stresses that result in rheological behavior that is quite different from that of simple Newtonian fluids. Near phase boundaries, shear can lead to dynamical instabilities and new structures in these systems.

Similarly, flow induced hydrodynamic stress on polymers or vesicles has a dramatic (and incompletely understood) influence on both the shape of these networks as well as the rheology of suspensions. For example, the deformation of polymers in hydrodynamic flows is a fundamental and still incompletely resolved problem in polymer physics, and the rheology and shape of red blood cells flowing in narrow capillaries is of great importance in medicine. Excess shear stress at the endothelial wall can lead to life threatening lesions called dissecting aneurysms. The shear stress at vessel walls also influences many other vascular functions such as the permeability of the vascular walls to large molecules, the biosynthetic activity of the endothelial cells, and the coagulation of the blood.

While there has been some success understanding these problems using analytic methods, progress has been hindered by the lack of efficient simulation techniques. What is required is a sufficiently coarse-grained description of the solvent degrees of freedom. A promising approach to this problem is to describe the hydrodynamic degrees of freedom using a Boltzmann equation, discretized in velocity, space, and time.

In this project, these researchers intend to develop and extend Lattice Boltzmann (LB) methods to study these systems. Some recent results of this work have already been published. Development of a LB scheme capable of describing the dynamics of all the hydrodynamic modes of a normal non-ideal fluid is currently underway.

Research Group

Thomas Ihle, Research Associate

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M. Germana Paterlini, Principal Investigator

Modeling of Receptors and their Ligands

Chemokine receptors are members of the large class of G-protein coupled receptors (GPCR) involved in signal transduction with which they share a homologous 7-helical transmembrane (TM region). These receptors are present in cells of the immune system and some are cofactors for human immunodeficiency virus-1 (HIV-1) viral fusion. The ligands for this receptor class, the chemokines, are

small proteins that contain 50 to 70 amino acids. These proteins, despite their similar folding motif, can show high selectivity toward their respective receptors. The chemokine receptors used by HIV-1, their protein ligands, and the binding of chemokines to the receptor models are all currently being studied.

Computational efforts focus on three areas. The first area deals with the construction of receptor models. Modeling of the transmembrane regions is performed using available structural experimental data, secondary structure prediction methods, and homology modeling techniques. In addition, a loop algorithm, combined with a knowledge-based conformational search, is used to construct the extracellular and intracellular loop regions. The model building makes use of previous results on modeling of the opioid receptor by exploiting the sequence homology in the TM region of these two receptor classes.

The second focus is on construction of the models of chemokines. The X-ray or Nuclear Magnetic Resonance (NMR) structures have been resolved for only a handful of chemokines. However, all these proteins share a similar folding motif. These researchers are making use of a sequence homology to construct models of additional chemokines. Known and modeled chemokines are compared by homology in the electrostatic potential surface to identify similarities that could aid in the docking of these chemokines to their receptors.

The last focus is on the binding of the chemokines to the receptor models. Complementarity between the shape and electrostatic potential surface of chemokines and receptor models is used to identify possible regions of association in the extracellular regions. The methodology is tested first on systems for which structural and mutagenesis data are available on both receptor and chemokine.

This research also deals with the modeling of opioid receptors. The opioid receptors are also members of the large class of GPCRs. The computational research of this group involves the construction and optimization of a three-dimensional model of the opioid receptors and simulation of ligand binding. These researchers have already studied the seven TM regions and part of the extracellular loop (EL) regions and are now modeling the remaining EL and intracellular (IL) regions connecting the helices. This is being used along with indirect structural information from site-directed mutagenesis data. Molecular dynamics simulations are then used to identify specific structural motions of the TM regions that can be correlated with receptor activation and signal transduction. The modeling efforts are being expanded to include those intracellular regions of the receptors that interact with G proteins.

Research Group

Thomas G. Metzger, Graduate Student Researcher

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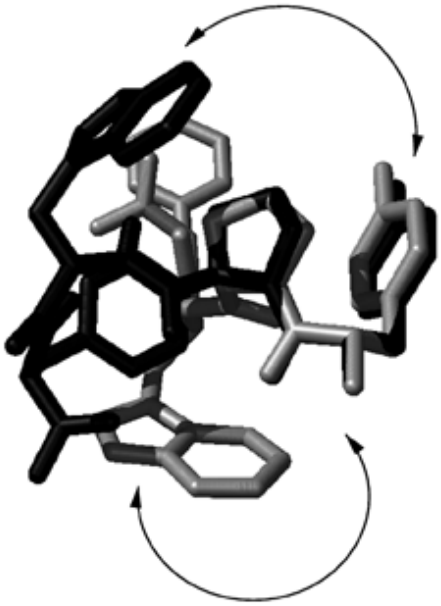
Philip S. Portoghese, Principal Investigator and M. Germana Paterlini, Co-Principal Investigator

Modeling of Opioid and Chemokine Receptors with their Ligands

The opioid receptors are members of the large class of G-protein coupled receptors (GPCRs) involved in signal transduction. This computational research involves the construction and optimization of a

three-dimensional model of the opioid receptors and simulation of ligand binding. Following recent experimental data of the GPCR rhodopsin, these researchers are currently refining the model of the 7-helical transmembrane (TM region) previously built. The extracellular and intracellular regions connecting the TM region are then constructed. These regions, from nine to twenty-five amino acid residues in length, are being studied using a combination of conformational search methods and homology modeling together with indirect structural information from site-directed mutagenesis data. Previously, they have been able to successfully dock the endogenous peptide dynorphin A to the kï¿½opioid receptor. Such binding involves residues in both the TM region and the second extracellular loop region. The remaining loops are then modeled. These researchers intend to use the structural models to study the mechanism of receptor activation. Previously, they postulated a mechanism of receptor activation by dynorphin, which involve rigid motion of the helices in the transmembrane helices. They are using molecular dynamics simulations to identify specific structural motions of the TM regions that can be correlated with receptor activation and signal transduction. The binding and activation of other endogenous ligands are then examined. The conformational properties of the opioid peptide endomorphins in condensed phase have already been studied. These computations are being extended to include binding of these peptides to the mï¿½opioid receptor.

Further computational efforts are being dedicated to develop models for chemokine receptors. These proteins are also members of the GPCR family and share one of the highest homologies with the opioid receptors. There is a strong interest in these proteins because they have been implicated in transmission of human immunodeficiency virus (HIV). It is known that opioids can modulate immune response, and the opioid and chemokine systems share several functional similarities. However, structural similarities and binding characteristics have not yet been studied and compared. Structural models of relevant chemokine receptors are being developed so they can be compared with that of the opioid receptors. Modeling includes both the TM and loop regions.



Endomorphin-1 is a newly discovered peptide of the m-opioid receptor. The binding properties of this peptide depend on the orientation of the aromatic residues. Professor Paterlini and Professor Porthogheseï¿½s research, in collaboration with Professor Ferguson, has determined the solution structure of this peptide and its biologically inactive analog using nuclear magnetic resonance spectroscopy and molecular dynamics simulations. The figure illustrates how stereochemical

substitution of proline with D-proline changes the relative orientation of the tyrosine and tryptophan side chains (left: endomorphin-1, right: D-pro-endomorphin-1). Comparison between the active and inactive forms of endomorphin-1 allows identification of the bioactive conformation of this peptide.

Research Group

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Bertrand Le Bourdonnec, Research Associate
Christopher R. McCurdy, Research Associate
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M. Germana Paterlini, Co-Principal Investigator
Shiv Kumar Sharma, Research Associate
William Stevens, Research Associate

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Carston R. Wagner

Anti-Tumor Catalytic Antibodies

Chemotherapy is a potent weapon in the clinical treatment of cancer. Serious side effects in most treatment is largely due to the lack of selectivity of highly toxic drugs for the target tumor cells over normal cells. Therefore, the design of targeted drugs or effective drug delivery vehicles is crucial to advancing cancer chemotherapy. These researchers are developing a novel and general strategy for the site-specific delivery of antineoplastic therapeutics that will rely on the design and optimization of targeted catalytic antibodies for the site-specific release of carbamate prodrugs of antitumor agents. Initial model studies are concentrating on the delivery of the well characterized antineoplastic agents.

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John H. Kareken, Principal Investigator

Comparison of Cox-Ingersoll-Ross Interest Rate Models

This work is comparing two- and three-factor Cox-Ingersoll-Ross (CIR) interest rate models in describing the evolution of the LIBOR yield curve over time. Cap and Swaption prices are used as bases for comparison.

The maximum likelihood estimation of both the two-and three-factor CIR models have been completed along with the computation of Cap and Swaption prices using the two-factor CIR model. Presently, computations are being done on the Cap and Swaption prices using the three-factor CIR model. Determining each Cap and Swaption price using the model involves computing many two-dimensional integrals (e.g., for the 10-year Cap price, there are 80 and for 10-year Swaption prices, there are 40 two-dimensional integrals to be computed). Furthermore, weekly prices must be computed for the two and a half year period in addition to each weekly 10-year Cap price and each weekly 3-month/10-year Swaption price.

Research Group

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Murugappa Krishnan, Principal Investigator

Information and Financial Markets

Research in financial markets has assumed that markets were perfect (agents take prices as given and can not be manipulated), and that all information was public. More recently, after the wave of insider trading scandals in the 1980ï¿½s, there is recognition that there are some big players who have access to private information and the ability to manipulate market prices. Most of this research is theoretical, and there is little evidence about elementary parametersï¿½like the precision of private information, the level of background noise in a financial market, and the variability of asset returnsï¿½that govern risk in such models. The research undertaken by these researchers is working to identifying such parameters. After identification, they work to measure how the financial market is manipulated by large traders and market makers. In the end, these researchers measure who gains and who loses.

Research Group

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Brian P. McCall, Associate Fellow

Development and Application of Life History Models in Economics

This research continues to apply newly developed statistical methods for life-history data to interesting questions in the economics of education and labor markets. Specifically, this research uses both single and multi-spell hazard and competing risks models that adjust for possible selectivity bias. These new methods are used to study the effect of unemployment insurance benefit levels on re-employment into jobs offering health insurance; gender, age, and race differences in re-employment behavior following job displacement; the effect of financial aid on the drop-out and graduation behavior of college students; whether delaying college enrollment after high school completion affects college completion; the effect of race and union status on job quitting behavior; and the occupational mobility of youths.

Many of these analyses involve policy simulations. New resources are being used to bootstrap the standard errors of these policy experiments. This group has shown that increasing certain unemployment insurance parameters increased the re-employment rate into part-time jobs. However, these estimates were just point estimates. By developing a program to bootstrap the standard errors, this group is able to calculate confidence interval estimates.

Previous analyses of life history data have assumed that spell or duration data is continuous. However, economic data is usually grouped. Therefore, duration data involves a numerous amount of ties; in the weekly unemployment duration data, a large proportion of individuals find jobs in the first week. Thus, statistical estimation techniques are developed specifically for grouped duration data.

Both the competing risks and multi-spell hazard models used in this research are flexible. In multiple spell hazard models, unobserved heterogeneity is accounted for by using a multi-dimensional, mass-point mixing distribution.

The competing risks model accommodates dependent risks by allowing for (possible correlated) unobserved heterogeneity to affect the latent marginal hazard functions. Again, a multi-dimensional mass-point mixing distribution is used to model such unobserved heterogeneity. Finally, the selectivity-corrected hazard and competing risks models employ multivariate mass-point mixing distributions. The benefits of such mixing distributions are that they yield semi-parametric consistent estimators when the number of mass points increase with the sample size, and they allow one to avoid the evaluation of multiple integrals in the likelihood function.
These estimation techniques are currently being applied to the continuing study of the effect of financial aid on college drop-out and graduation behavior using administrative data from the University of Minnesota. A new cohort of data has been acquired that better tracks the financial aid application behavior of students over time.

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Department of Operations and Management Science

Michael R. Taaffe

Michael R. Taaffe, Principal Investigator

Process Management of New Product Development Projects: An Application to Stochastic Network

There is growing pressure on firms to accelerate the development and launching of new products. Consequently, firms are faced with the problem of managing many concurrent new product development projects that place competing demands on shared human and technical resources. This problem is further compounded by the uncertainty inherent in product development. This study aims at developing and implementing a modeling framework for analyzing product-development time in organizational units pursuing multiple concurrent non-unique projects using shared resources. The modeling framework is conceptually founded on a process view of the development projects. Each project involves unique challenges that require unique solutions. However, many tasks and sequences of tasks are the same across projects. Process management of product-development projects exploit similarities through standardization and continuous improvement without destroying creativity. This framework makes it possible to reveal the structure of the development process, identify and assess ideas for reducing development times, and achieve a balance for an organizational unitï¿½s capacity and workload.

Research Group

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Daniel D. Joseph
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Thomas S. Lundgren
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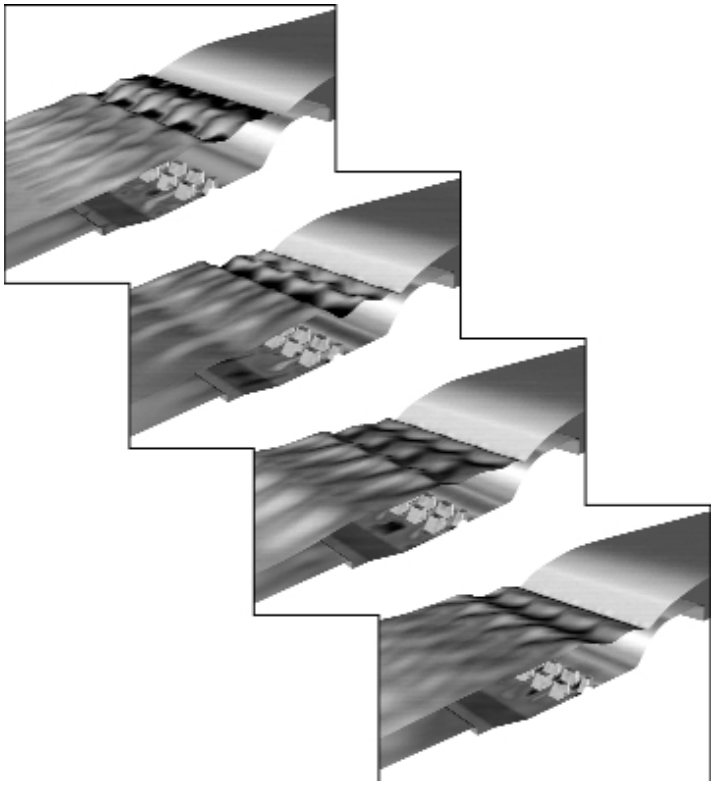
Marek Behr, Principal Investigator

Portable Message Passing Implementations of Computational Fluid Dynamics Code

This work is developing effective simulation methods for unsteady flows of fluids in situations involving significant deformations of the computational domain. The methods are based on the finite element technique, using stabilized formulations, complex unstructured three-dimensional meshes, and iterative solution strategies. The parallel implementation is based on message-passing communication libraries such as message passing interface (MPI) and parallel virtual machine (PVM), and this implementation is portable across a wide range of machines. The two sets of problems under current investigation center on free-surface flows and on translating and rotating geometries that can be modeled using the Shear-Slip Mesh Update Method (SSMUM).

In free-surface flows, location of the interface is not known a priori, and it needs to be determined as part of the overall solution. The major challenges in these types of simulations are accurate representation of the interface in long-term time-integration, devising mathematical models and computational methods that take large variations of geometric scales into account, and keeping the computational cost at an acceptable level. Wave formation and breakup are also among the challenges. The mathematical models created by these researchers are based on the Navier-Stokes equations of incompressible flows. Depending on complexity of the interface and other conditions, this group is developing two different methods. In one approach, they are developing a stabilized space-time finite element formulation, which is an interface-tracking method with moving mesh. In another approach, they are developing a stabilized finite element/interface-capturing formulation with fixed meshes. The interface-capturing method is more flexible but yields less accurate representation of the interface compared to the interface-tracking method. The interface-tracking method has been successfully extended to three-dimensional and periodic flows. A model of the Olmsted Dam on the Ohio River is now being used as a test problem.



Flow in a spillway of a dam: Free-surface position and velocity filed at four instants.

Research Group

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Graham V. Candler, Fellow

Simulation of Reacting Flows

Recent experiments performed in the California Institute of Technology Shock Tunnel have shown hypersonic boundary layers to be stabilized by reactions that occur in the flow field. The result is that transition to turbulence in the boundary layer is delayed, reducing the aerodynamic heating and drag. If this effect can be understood, it would change the way future hypersonic aircraft and planetary entry spacecraft are designed.

Recently, these researchers performed calculations using linear stability theory that confirmed the stabilizing effect shown in these experiments. Calculations show that energy-absorbing chemical reactions tend to reduce the growth of disturbances in the sharp-cone flows studied in the experiments. Conversely, energy-releasing reactions destabilize the flow and cause transition to occur more readily. Calculations also show that the stabilizing effect does not occur under all conditions or geometries. These calculations are continued in an effort to gain a better understanding of the chemistry-transition interaction.

A family of implicit computational fluid dynamics methods for simulation of high-temperature reacting flows has been under development in the Department of Aerospace Engineering and Mechanics at the University of Minnesota. These methods were designed for straight-forward implementation on conventional massively parallel computers. The methods have efficiently yielded steady-state solutions to many test problems on several widely different machines. Very good single-node, floating point performance was obtained on these machines with excellent parallel efficiency.

One method under development uses a series of simple pointwise matrix operations rather than complicated linear algebra to approximately solve the implicit operator. In essence, this requires many nearest-neighbor communications on a regular grid. This can be implemented very efficiently in data-parallel FORTRAN90, and on the other parallel machines used, it is easy to hide communication costs with asynchronous message-passing routines in message passing interface (MPI).

When these methods are tested and optimized, they are used to simulate a wide variety of reacting flows. These include simulations of planetary entry flows, rocket motor plumes, jet interaction flows, atmospheric pressure plasma flows, and hypersonic turbulent boundary layers. Overall, this work is helping develop a greater understanding of how finite-rate chemical reactions interact with fluid motion.

Additional work using direct numerical simulations and large-eddy simulations of turbulence is being

done on compressible turbulent flows. Two major classes of flows are being studiedï¿½turbulent supersonic compressible boundary layers and chemically reacting turbulent flows. Two new methods to reduce the cost of performing these simulations are also under development. First, these researchers are continuing the development and testing of a time accurate implicit method shown to reduce cost by a factor of at least five. Second, a new grid blocking idea is implemented to reduce the computational cost by an additional order of magnitude. These new methods are being used to perform the first simulations of compressible turbulent boundary layers that include the presence of chemical reactions and shock waves. The work is helping to increase the understanding of these important flows and is providing a new database of statistically exact flows for turbulence model validation and calibration.

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Large Deformation in Nonlinear Elasticity and the Thermomechanics of Propagating Phase Boundaries

The nonlinear theory of elasticity is more appropriate for the investigation of coexistent phase phenomena and singular behavior in the mechanics of materials than its linear counterpart. In the nonlinear theory, the governing system of equations can support the possibility of changes of type for certain applications that are not possible in the linear theory. Often, this is associated with the phenomena of instability and bifurcation, which leads to highly localized, large deformations. For solids, there are contemporary computational developments, iteration procedures, adaptive methods, and continuation techniques already being used successfully in the computation of regular boundary value problems that arise from such nonlinear theories. Some of these ideas are being used in investigations by these researchers, but the emphasis of this program is on the role of singularities in

problems where solutions are not regular. The injectivity of the deformation map is of great concern here.

Purely mechanical theories of phase transitions require admissibility hypotheses (kinetic relations) to be solvable. These kinetic relations, while ensuring uniqueness, have questionable physical justification. These researchers propose that a thermomechanical model including capillarity, viscosity, and thermal conductivity is the appropriate setting, and it is the preferred framework for their investigation. Because the free energy is nonconvex, the governing equations are of mixed typeï¿½hyperbolic in regions of pure single phase and elliptic in the intervening spinoidal region. Continuing computations and analysis show this to be a promising method of calculating dynamic phase transitions. However, further investigations, including the determination of dependence on numerical methods, are being pursued. Currently, the researchers are implementing and testing several finite element methods for solving these equations, and they are developing their own approach. Part of the problem is in optimizing the computations and addressing the questions of parallelization and alternate numerical techniques.

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Molecular Simulation for Investigating Crazing of Linear Polymers

Under stressing, strained polymer structures become damaged. The damage may appear in various forms as yielding, cavitation, flow, molecular orientation, crazing, or a combination of several possibilities. The most important of these possibilities is crazing, which is not easily studied with computer modeling techniques. However, after a long and careful search, a new method of approach has been found. Instead of employing the usual low-energy minimization process, a high-energy minimizing method has been developed for obtaining the initial guess of a polymeric model molecular structure for the potential energy minimization and analyses. It appears that the new method can yield useful and significant information on crazing. When the individual bonding units in a fundamental model cube are examined, several bonding energies are capable of exceeding their respective activation energy levels. This suggests the possibilities of the cessation of the primary bonds in the molecular structure and the initiation and inception of crazing. As a result, the crazing of polypropylene has been partially studied. It is hoped that this new method can be applied to the study of the polystyrene polymer molecules to explore reasons for their ease of crazing behavior.

Research Group

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Direct Numerical Simulation and Modeling of Solid-Liquid Flows

Under a new National Science Foundation grant, this group is continuing their work in developing scalable, highly efficient parallel finite-element codes (particle movers) for the direct numerical simulation of the motion of solid particles in Newtonian and viscoelastic fluids. To carry out such simulations, the group must solve coupled initial value problems for the fluid and particle motions. In these problems, the particle motions are governed by equations of rigid-body motion with hydrodynamic forces and torques on the right-hand side.

These researchers have developed two separate particle movers. The Arbitrary Lagrangian Eulerian (ALE) particle mover is based on a generalization of a standard Galerkin finite-element method. It uses an unstructured body-fitted mesh and an ALE scheme to handle the time-dependent domain of the fluid flow. A new mesh is generated when the old one becomes too distorted, and the flow field is projected onto the new mesh. The Distributed Lagrange Multiplier (DLM) particle mover is based on a fictitious-domain method in which the fluid is imagined to fill space inside the particle boundaries, and the rigid-body motion inside the particles is enforced via distributed Lagrange multipliers. The DLM particle mover uses a fixed, regular mesh over the entire fluid-particle domain. Both schemes are based on a combined fluid-particle weak formulation from which the hydrodynamic forces and torques have been eliminated. Both particle movers have been parallelized, and both movers are running simulations with up to one thousand particles in two dimensions and up to one hundred particles in three dimensions.

These researchers are also developing a Lagrangian particle tracker for solid-liquid flows. This scheme does not solve the exact equations of solid-liquid flow; it is based on a two-fluid model equation in which the fluid and solid velocities and the solids fraction are unknowns. The particles influence the motion of the fluid through a momentum exchange term, and an empirical form of the hydrodynamic forces act back on the particle through Newton's laws. This scheme allows computations of motions of tens of thousands of point particles to be completed.

Presently, these researchers are improving the parallel performance of their particle movers using block preconditioners that take advantage of the structure of the governing equations. They are also developing matrix-free methods that allow larger problems to be solved. A viscoelastic version of the DLM particle mover has been developed. In addition, computational investigations into the fundamental dynamics of fluid-particle motions are being continued using the particle movers. This group has also begun a series of investigations on the problem of effective sand transport in fractured oil reservoirs. The results of these studies will have a major impact on the efficiency of enhanced oil recovery operations.

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

This research is developing a computational method to predict microstructural features in alloys. Such a tool would allow metallurgists to develop new alloys with new properties. Microstructure is a critical variable in alloys as it sets the macroscopic mechanical properties of an alloy. The microstructures being studied arise from a solid-state diffusional transformation in multicomponent alloys. The transformation occurs when the temperature of the alloy is abruptly lowered, and a thermodynamically stable single phase separates into multiple phases at these lower temperatures. This separation involves diffusion of matter among the distinct crystal phases, surface energy at the interfaces between the phases, and elastic energy.

One main issue in studying microstructure is to prevent the in situ degradation of material properties that occur by a coarsening process. This process occurs when a dispersion of very small precipitates evolves to a system consisting of a few very large precipitates in order to decrease the surface energy of the system. This coarsening severely degrades the properties of an alloy and is especially important in high-temperature applications such as jet turbine blades. It has been speculated that elasticity can lead to inverse coarsening in which small particles grow at the expense of large ones and material performance would improve with time.

This work involves understanding the interactions among diffusion, elastic stresses, and surface energy. Previously, this group successfully used boundary integral methods, based on sharp interfaces, to study growth and coarsening in elastically isotropic and orthotropic inhomogeneous systems. They included surface energy anisotropy and investigated the interaction between the surface energy and elastic anisotropies. They developed interface (Cahn-Hilliard type) formulations for some of these problems.

Continuing work includes looking at elastic stress effects in inhomogeneous anisotropic systems where

the microstructure consists of many 2nd-phase precipitates. This involves looking at realistic alloy systems such as steels and nickel superalloys. The researchers use both the boundary integral methods (BIM) and diffuse interface methods (DIM) to study the coarsening (evolution) process. In the BIM, the field equations for composition and elasticity are mapped to the sharp boundaries between the phases, and the boundary conditions are used to formulate boundary integral equations. These equations are solved, the resulting velocities of the interfaces are computed, and the interface position is updated. The most time consuming part of this calculation is the solution of the integral equations for the elasticity fields. The current focus is on more efficient techniques to solve these systems. In the DI approach, the evolution of the smooth fields is given by a coupled set of partial differential equations, solved using spectral methods to follow the entire evolution process. The DIM for anisotropic, inhomogeneous systems is being developed.

In this work, the group is continuing to generate realistic simulations of microstructure evolution in solids. The thrust of the research includes crystalline effects such as elastic anisotropy (multiple precipitates), ordering, and strain-induced phase transformations. In the latter two cases, long range diffusion will no longer be the rate controlling step in the precipitate evolution process, and the crystallography of the systems will play a much more important role in the evolution.

Research Group

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Thomas S. Lundgren, Principal

High-speed Turbulent Jets

This research is studying aeroacoustic noise generation in a supersonic round jet. Understanding the effect of turbulence structure on the noise without numerically comprising the turbulence is of particular interest. This requires direct numerical simulations (DNS). In order to use DNS at high enough Reynolds numbers to get sufficient turbulence structure, these researchers have solved the temporal jet problem using periodicity in the direction of the jet axis. Physically, this means that turbulent structures in the jet are repeated in successive downstream cells instead of being gradually modified downstream into a jet plume. In order to answer some questions about the turbulence, they must partially compromise the overall structure of the jet.

Numerical results using B-splines in the radial direction and spectral expansions in the axial and azimuthal directions have been carried out for a Mach 2 jet with swirl. The results show turbulent structure very similar to what is found for low speed jets. This work has been computed; the results can be found in the Ph.D. thesis of Dr. Ram Rao, and a paper summarizing these results has been submitted for publication.

A new project on fuel spray combustion has been started. In the numerical analysis of sprays, fuel

sprays in combustion chambers in particular, one attempts to track the motion of drops through the surrounding turbulent gas flow. When the relative velocity of the drop becomes large, hydrodynamic forces can cause the drop to break up into a number of smaller drops, and the analyst must track these daughter droplets. There is an existing method for predicting the breakup called the Taylor Analogy Breakup model (TAB model), which is based on an analogy between an oscillating droplet and a spring-mass linear oscillator. This project is placing the TAB model on a firmer footing through more complete analysis of the fluid dynamics of this two-phase system. Basically, when a drop finds itself in a high-speed flow, the high-impact pressure at the front and rear and the Bernoulli suction around the equator tend to squeeze the droplet into a lens-shape. These forces are resisted by the surface tension and inertia of the drop. This problem can be analyzed numerically by means of a boundary integral method in which the potential flow of this two phase system is modeled by superimposing dipoles along the interface between the two fluids, solving for the shape by a Lagrangian method that follows surface marker points in the velocity field induced by the dipole distribution.

Research Group

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Optimal Helicopter Flight Paths in One Engine Failure

This research uses trajectory optimization methods to study helicopter flight operations in the event of one engine failure. Engine failure represents a major factor in helicopter accidents and incidents. The Federal Aviation Administration (FAA) classifies transport helicopters in two categories according to their characteristics in engine failure. Category A helicopters must have the ability to continue flight in the event of one engine failure. Category B helicopters are only required to land safely in such cases. As a result, only Category A helicopters are allowed to operate from city-center building heliports, oil rigs, and remote areas where no emergency landing site is available. Appropriate flight strategies in the event of one engine failure have been determined conventionally from flight tests. These are very expensive and time-consuming. Furthermore, recommended maximum takeoff weights and runway requirements from flight tests are very conservative. Past studies have used point-mass helicopter models. While these models are useful in describing energy relationships in a helicopter flight, a rigid-body model is necessary to determine helicopter attitude angles such as pitch and roll. The rigid-body model helps to develop guidance variables that a pilot can use in real flight as well. With this in mind, these researchers have developed a three-dimensional, six degree-of-freedom, rigid-body model. It consists of thirteen state variables, four control variables, and several control parameters. There are thirteen differential equations and many constraints on functions of states and controls. Overall, this model allows these researchers to conduct extensive optimization studies to determine optimal flight paths.

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Robert W. Carr, Principal Investigator

Microcanonical Transition State Theory Rate Coefficients from Thermal Rate Constants via Inverse Laplace Transformation

On the basis of concepts from the mathematical theory of the approximation of functions, this group proposes a method of deriving microcanonical transition state theory rate coefficients, as a function of both the total energy and the total angular momentum, from thermal dataï¿½namely, the limiting high-pressure rate coefficients. The method does not require the knowledge of the frequencies and degeneracies of the transition state and is general in that it allows for non-Arrhenius forms of temperature dependence of the rate coefficients, but it only applies to reactions possessing an intrinsic energy barrier. It is shown that the derived microcanonical rate coefficient is almost identical to the computed Rice-Ramsperger-Kassel-Marcus (RRKM) microcanonical rate coefficient using explicit frequencies and degeneracies of the transition state, and that the difference between the two is uniformly distributed over the entire range of total energy and the entire range of the total angular momentum. The microcanonical rate coefficients from the proposed method are compared with those from a standard non-variational RRKM calculation for the unimolecular decomposition of the ethyl radical and the unimolecular isomerization of methyl isocyanide. The agreement is excellent. The fine structure of the microcanonical rate coefficient near the threshold of the reaction is analyzed, and the difficulty of extending the method to obtain variational microcanonical rate coefficients is described.

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High Performance Algorithms for Electronic Materials

These researchers are continuing their investigations on dielectrics with emphasis on silica and related materials as well as on semiconductors. A major part of the program is to develop new methods and algorithms for examining the electronic structure of large systems. They have developed some new procedures for determining the structural and electronic properties of localized systems such as clusters, quantum dots, and point defects. In general, the applications focus on complex systems with numerous atoms and many degrees-of-freedom.

Silicon is the material of choice for making electronic devices because its oxide is electronically inert. These researchers are currently examining defects in silicon dioxide to understand how this oxide can be further improved. Current device technologies use oxide layers as thin as ~20 ï¿½. For layers this thin, understanding intrinsic defects become increasingly important. The current focus is to determine the electronic properties of oxygen vacancies and interstitial oxygen atoms.

Another emphasis in this area deals with electronic and structural properties of complex solids. This group has initiated an effort to examine AlPO4 (a-berlinite). This material amorphizes under pressure; however, it exhibits a memory effect. Upon release of pressure, berlinte re-crystallizes with the same orientation it possessed before the amorphization transformation. Calculations on this material have been completed, and new calculations on a related material (GaAsO4) have been started.

The second part of this research focuses on electronic and structural properties of semiconductors. One focus is on liquid semiconductors. These researchers have developed molecular dynamics simulation techniques based on ab initio pseudopotential methods. The pair correlation function, electronic density of states, and the electronic charge density have been calculated for a number of liquids. The method is being used to examine liquid CdTe, which presents some fundamental challenges.

These researchers have also examined the behavior of semiconductor clusters at finite temperature and compared them to recent photoemission data. This is one of the few available calculations where experiment may be compared directly to theory. More recently, they have examined the polarizability of small clusters.

The final emphasis of the research, in collaboration with Co-Principal Investigator Yousef Saad, is on quantum dots. In this work, the researchers have considered large clusters of silicon. These clusters have very different optical gaps than crystalline silicon. The role of size can be used to change the gap of silicon in order that it be used for optical devices. Crystalline silicon has a band gap with poor radiative efficiency in the visible spectrum. Most experiments on quantum dots are on systems larger than can be handled by standard theoretical methods (the smallest dot measured is about 600 atoms). By implementing their real space methods, these researchers were able to consider clusters up to one thousand atoms.

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John S. Dahler, Associate Fellow

Colloidal Dispersion, Liquid-Phase Dynamics, Chemically Reactive Fluids, and Atomic Collision Processes

This research combines five projects. The first project focuses on vibrational relaxation and reactive liquid phase collisions. There is considerable evidence indicating that solvent complexes play an important role in the photochemistry of iodine in dense fluids. To further understand the effects of these complexes on iodine photochemistry, these researchers need to determine the electronic states of the complex because fragmentation of the complex leads to an electronic transition of the iodine molecule. The technologies developed for the vibrational relaxation problem are used to examine other aspects of iodine photochemistry in dense fluids. A picture of how various aspects of photochemistry fit together is gradually emerging.

The second project focuses on kinetic theory of colloidal and polymeric solutions. Fluid mechanical properties of colloidal suspensions are of vital concern in a large number of practical, industrial applications. However, until very recently, the only theories capable of accounting for these properties were limited in their applicability to very dilute solutions. The theory these researchers have developed, and which is now the object of numerical tests, is not subject to such constraints. Preliminary calculations indicate that it works well. Proposed computations test the sensitivity of the theoretical predictions to a variety of parameters, characteristic of the particle-particle forces.

The next focus is on kinetic theory of a fluid composed of simple reactive spheres. Theoretical analyses of the scattering of light and acoustical disturbances from chemically reactive fluids have invariably been based on continuum mechanical models of the reactive processes. In contrast to this, the theory used in this research invokes a simple, but much tested, molecular scale model for the chemically reactive events. The theory is designed to generate a multitude of wavenumber and frequency

dependent correlation functionsï¿½some that can be compared directly with the results of experimental measurements of slow-neutron and quasi-elastic light scattering. The computational output includes a wealth of information about the frequency and wave length dependence of the familiar hydrodynamic and other modes.

The fourth project deals with newtonian viscosity of moderately dense suspensions. This group has developed a theory from which it is possible to compute the viscosity of a suspension as a power series in the volume fraction of the solute species, ÿ. Explicit formulas have been derived for the series coefficients associated with the first and second powers of ÿ. Values obtained from these formulas agree with the outputs of earlier theories for hard spheres with stick-slip boundary conditions. However, this theory is applicable to a broader class of solute-solvent interactions than the earlier theories and to suspensions of nonspherical solute particles as well.

The last project focuses on applications of a new renormalization group (RG) to a variety of physical problems. The researchers have invented a RG that differs from the generalized propagator group upon which most previous RG calculations have been based. This group has been designed to deal specifically with functions that are positive valued. This group and an associated Lie algebra computational algorithm can be applied to a wide variety of physical systems.

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Dynamics and Control of Chemical Plants and Feedback Control of Incompressible Flows

Designing effective controllers for complete chemical plants has attracted considerable attention, owing in part to benchmark industrial problems. A typical chemical plant consists of a set of chemical reactors, a collection of separation units to separate reactants and products, and one or more streams from the separation units to the reactors to recycle unconverted reactants.

These researchers are developing a systematic framework for designing controllers for complete chemical plants and testing the proposed control schemes through simulations of detailed dynamic models of the plants. To this end, they establish that chemical plants with recycle exhibit a non-explicit, time-scale multiplicity. This implies that the control objectives should be properly formulated and addressed in the appropriate time-scales. More specifically, in the fast time-scale, dynamics of the individual units evolve independently of each other with weak interactions arising from the recycle. These weak interactions can be ignored in the design of distributed controllers to achieve the requisite stabilization/tracking objectives for individual units in the fast time-scale. However, these weak interactions between the individual units give rise to a significant dynamics of the plant core. This

indicates that a separate supervisory controller should be designed to address overall plant control objectives of production rate, product purity, and so forth in the slow time-scale.

Two key features guiding design of the supervisory controller for the slow plant dynamics are that these slow dynamics are usually of low order and highly nonlinear. Thus, it is imperative to perform a systematic model-reduction to obtain a low-order model describing the essential slow dynamics of the plant core and useful for nonlinear controller design. Such a model can be obtained by ignoring the fast dynamics of individual units with the respective distributed controllers. The resulting model is given by a high-index differential and algebraic equation system. For such systems, a controller can be designed on the basis of an approximate minimal-order state-space realization.

Of equal importance is dynamics and control of fluid flows in the context of materials/chemical processing applications. Incompressible, isothermal flows are mathematically represented by time dependent momentum equations and the continuity constraint. Difficulties associated with this representation, known as the velocity-pressure formulation, are continuity constraint, nonlinear convection term, and absence of an explicit equation for pressure.

This work studies the dynamics and control of incompressible flow in a two-dimensional driven cavity. Current work focuses on spatial discretization of velocity-pressure formulation via finite differences and the Galerkin Finite Element Method. To this end, researchers address the derivation of reduced-order ordinary differential equation model that captures the dynamic behavior of the process using the Fourier-Galerkin method with the stream-function formulation. Accuracy of this reduced-order model is evaluated through comparisons with the model obtained via a finite difference discretization of the velocity-pressure formulation. This model is used as the basis for a detailed computational study of the dynamics of the system. Finally, the problem of controlling the flow pattern in the cavity is addressed.

Research Group

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H. Ted Davis, Fellow

Fluid Physics for the Technologies

This work is capitalizing on unique research opportunities, either to address important issues arising from ongoing research or special short term collaborative opportunities.

The first project concentrates on first principles molecular dynamics (FP-MD) algorithms for the study of zeolites and related aluminosilicates. The work centers around studies of zeolites utilizing a state-of-the-art FP-MD with variable cell shape (VCS). It self-consistently solves the electronic structure of the system at every time step of the dynamics in order to give an accurate representation of the interatomic bonding. This version of MD goes beyond previous implementations by introducing strains in the simulations and removing essentially all structural constraints. This particular feature makes it ideally suited to investigate the behavior of unisotropic materials at a wide variety of temperatures and

pressures. The first step in the work is the calculation of charge densities and the electronic band structure of several zeolites by direct minimization of crystal structures. Further FP-MD studies quantify the acid/base characteristics of adsorption sites as well as provide qualitative insight into the adsorption process. A simple structure of thirty-six atoms per unit cell is being used as a benchmark of the planewave formulation of the group's method versus recent periodic Hartree-Fock methods.

Another project deals with a fundamental study of configurations of non-spherical shaped molecules in nano-spaces. Molecules confined to nano-spaces behave differently than in their bulk environments. At room temperatures and pressures, compounds that are normally gases show liquid like densities inside nano-pores of zeolites. This difference is due to the increase in molecule-molecule interaction forced in the presence of the attractive well of the zeolite pore. Under such conditions, the properties of the fluid phase is influenced strongly by the way they pack. The group is working to understand the fundamentals of the molecule-pore and molecule-molecule interactions that are the basis of these phenomena; thus, forming a basis to predict behavior of different molecules in varied pore structures. They use statistical mechanics and simulation tools to virtually run experiments and study the system under various real and hypothetical conditions.

Further work is being done on the validation of Lattice Boltzmann hydrodynamics in complicated geometries. This method is being applied to study flow problems in porous media. To study the accuracy of the Lattice-Boltzmann method, the results are being compared against results obtained using FIDAP code.

The last project being worked on deals with molecular dynamics studies of the rate of evaporation of water from molecular clusters. This group is verifying the assumptions underlying the original ï¿½classicalï¿½ theory and a thermodynamics based theory with MD simulations. The model system consists of a thirty to one hundred molecule cluster of water molecules surrounded by a vapor phase of Lennard-Jones (LJ) molecules in the role of carrier gas that acts as a thermostat for the latent heat of evaporation or condensation of water molecules. The Nose thermostat is employed for the LJ phase; the water sub-system is run microcanonically. This system is contained by soft repulsive walls in three dimensions, positioned at a large distance compared to the cluster size. The tendency of the cluster to accept or lose a molecule is then investigated as a function of the number of constituent molecules. This helps to shed light on the critical cluster size.

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Jeffrey J. Derby, Fellow

Materials Processing Fundamentals

The overall objective of this research group is the application of large-scale numerical simulation to better understand the processing of advanced materials. All processes involve the interaction between continuum transport phenomena and the development of a solid-state material characterized by features that are both macroscopic and microscopic. To study phenomena that characterize these processes, the researchers solve free- and moving-boundary problems involving incompressible fluid dynamics, heat and mass transfer, chemical reaction, and interfacial physics via the finite element method.

One objective of this work is the development of algorithms to model materials processing systems. Current work focuses on massively parallel implementations of finite element methods, the development of moving boundary techniques for three-dimensional problems, better preconditioners to be used with iterative linear systems solution, parallel direct solvers, and implementation of advanced formulations for strongly nonlinear flows and transport.

Another objective is the study of crystal growth systems. Continuing effort has been directed at understanding several systems of interest. Current and future work focuses on the Czochralski growth of oxide crystals such as yttrium aluminum garnet (a laser host material) and lithium niobate (an acousto-optical material), the Bridgman growth of cadmium zinc telluride (a radiation detector material), and the solution growth of potassium titanyl phosphate (a nonlinear optical material). Specific work focuses on the description of molten and solid cadmium telluride, using atomistic methods to better understand its peculiar properties during crystal growth. A new project addresses important aspects of three-dimensional continuum transport phenomena occurring in microgravity crystal growth experiments. Another new project is developing a mesoscopic phenomenological model for step dynamics during the growth of a faceted crystal grown from the solution phase.

A third objective of the work is the study of sintering phenomena in ceramics systems. This group has successfully modeled the viscous sintering of simple configurations of particles. Work on modeling the sintering of polymeric materials, vacancy diffusion phenomena (which dominate the sintering behavior of crystalline materials), and to extend analyses to more complicated, three-dimensional particle arrangements.

Further work is being done on the development and application of algorithms for analysis of materials processing systems. The researchers are currently working to develop, implement, and test parallel algorithms designed to solve coupled systems of nonlinear partial differential equations (PDEs), which arise in mathematical models of materials processing systems under the assumption of the continuum physics. For instance, crystal growth of large single crystals, viscous sintering of ceramic particles, and microwave heating of foods. The algorithms are designed to compute approximate solutions of PDEs by second-order accurate mixed finite element methods, solve large systems of nonlinear algebraic

equations, and construct solution curves associated to naturally appearing model parameters.

Research Group

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Modeling of Micro- and Nanoindentation of Solidified/ Solidifying Polymeric Coatings

Solidified/solidifying polymeric coatings are widely used in many engineering applications because they can provide resistance to corrosion, reduce friction, and provide enhanced magnetic, optical, and mechanical properties. Micro- and nanoindentation and microscratch tests are commonly used techniques for measuring the mechanical properties of thin film/substrate systems. Although these tests can provide indentation hardness, adhesive strength, and driving force, some quantities such as the extent of the plastic zone, the residual stress distribution, and the permanent deformation field cannot be measured and must be determined numerically.

The current research is developing numerical models and viscoelastic indentation theories in support of the experimental work on micro- and nanoindentation currently being carried out in this group. The numerical model is expected to provide a better understanding of the mechanical properties of coating/substrate systems, and the theory is providing an essential way to interpret the indentation data. At the same time, results from numerical modeling can be used to optimize the experimental process and to provide an alternative tool for designing thin film/substrate materials in industry.

Micro- and nanoindentation process for thin film/substrate systems is classified as normal contact problems while microscratch process falls in the sliding contact category. The contact area, contact pressure, and scratch distance vary with the external load and are unknown prior to analysis. However, the compatibility condition of the contacting surfaces and a friction law must always be satisfied. These factors make contact problems complicated issues even when the simplest constitutive relation is

applied to the thin film/substrate materials.

Application of the finite element method in these two kinds of problems is cumbersome because the mathematical treatment becomes complicated for large deformations and because an implicit computational scheme requires the use of very large matrices, particularly for the three-dimensional problems of principal interest in this research. To overcome these limitations, a numerical model based on the explicit finite difference method has been developed. This numerical procedure allows large displacement, large deformation, and large sliding and elasto-plastic contact problems to be treated in an efficient manner in both two and three dimensions.

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Study of Hepatocyte Spheroid Formation, Modeling Plant Somatic Embryos, and Parallel Deconvolution of Confocal Microscopy Images

This first project in this research is a mechanistic study of hepatocyte spheroid formation. Liver parenchymal cells, like hepatocytes, can be isolated from rat or pig in situ and then be cultivated as monolayers. If these hepatocytes are plated onto surfaces with moderate adhesiveness, their locomotion can lead to agglomeration of cells into spheroids with diameters ranging from 80 mm to over 150 mm. Cells within these self-assembled structures typically exhibit a cytoarchitecture resembling the one of in vivo liver.

The aim of this project is to examine the structure-function relationship of spheroids and to investigate the mechanism of self-assembly by liver cells into organized tissue. The hypothesis is that tissue-like structures of hepatocytes are formed through the interplay of surface adhesiveness, intercellular ligand-receptor interaction, and mechanical force exerted by cell movement. These researchers are studying the kinetics and dynamics of cell-cell versus cell-surface forces during spheroid formation of hepatocytes from planar surfaces as a model of tissue-assembly. The process of agglomeration of hepatocytes into patches is analogous to the agglomeration of droplets of viscoelastic fluid on semi-wettable surfaces. Thus, a computational framework used in fluid mechanics is appropriate here. The modeling includes conservation equations for the cells and the substrate as well as equations that describe the mechanical cell-cell and cell-surface interactions.

The second project focuses on modeling the development of plant somatic embryos and plant shoot

tips. These researchers are studying the dynamics of growth and development by computer simulations of a mechanochemical model. They have shown that the model can represent the general trends of morphological change. Currently, they are studying embryo interactions. The model is being extended to simulate leaf bud initiation at plant shoot tips. Through the study, they are drawing conclusions on mechanistic similarities of embryo and shoot tip growth.

Validation of this model with experimental systems requires an unbiased classification system to group embryos into various morphological classes. An image acquisition and processing system has been developed to capture embryo images and generate a corresponding set of Fourier and size features. Classification of this multivariate data set is being carried out by statistical analysis.

The last project is concerned with parallel deconvolution of confocal microscopy images. Although a confocal microscope is designed to obtain data related only to the focal plane scanned, out-of-focus information can not be excluded during acquisition. Deconvolution techniques offer a solution to this problem, and parallel computing allows real-time image analysis and reconstruction. The researchers have implemented constrained iterative deconvolution methods. These are the most efficient for the case. Van Cittert's linear method and Gold's non-linear method have been applied in a parallel form on the confocal microscopy data. Removal of out-of-focus information revealed more structural and functional details, and the amount of processing time was substantially less compared to serial deconvolution of smaller data sets using the same methods. Currently, these researchers are developing filters to reduce the build-up of noise during the iterations. They are also working to eliminate the introduction of noise during the computational procedure.

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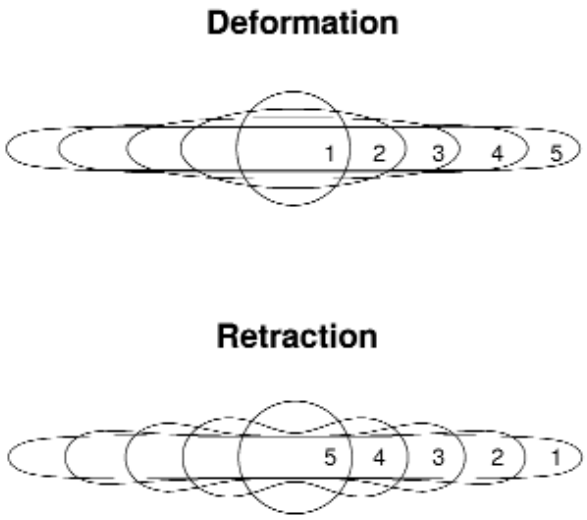
Three-Dimensional Modeling of Drop Deformation in Simple Shear and Extensional Flows

Recent experimental work has revealed that viscoelastic drops suspended in another viscoelastic

medium tend to flatten considerably when exposed to shear flow. This model of area generation is a means to more easily create polymer barrier materials among other possible applications. These researchers are exploring this phenomenon from a fluid dynamics approach by solving the governing transport equations using the finite element method (FEM). The key features and challenges of the problem include full three-dimensionality, two-phases, one or both phases being viscoelastic, time-dependent flow, and the drop shape defined by a moving boundary. While FEM is ideally suited to such a problem, difficulties arise in choosing or developing a numerically stable variation of FEM that allows for large departures from Newtonian fluid behavior. In addition, the three-dimensional aspect of the problem requires special attention to deal with problem size and computation time.

Recent work has been done to address the issues of two-phases, viscoelasticity, time-dependence, and moving-boundary accounting. These efforts have been directed toward flow problems involving an axis of symmetry that allows a three-dimensional problem to be treated using two spatial variables. While final results are forthcoming, preliminary results suggest that finer meshes are needed to resolve detailed features of the flow in regions of high curvature. In light of this, the final task to be undertaken, that of going from two-dimensional (actually three-dimensional axisymmetric) to fully three-dimensional, requires a significant increase in memory and the use of a parallelized matrix solver.



Deformation and retraction of a polymer drop subjected to uniaxial extensional flow. The dynamics are influenced by the complex fluid behavior of both the inner and outer fluids.

Research Group

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Homogeneous Nucleation Kinetics for Super-Saturated Molecular Vapors

This research is predicting the rate of nucleation of a condensed phase from a supersaturated molecular vapor. The systems of interest include molecules with cubic point group symmetries because the interaction potentials for such molecules are simpler than for arbitrary molecules, and these molecules often display multiple solid phases. As a first step in this process, these researchers are working to infer constraints on the orientation-dependent portion of the intermolecular potential from crystallographic data available in the Cambridge Structural Database, accessible through the Supercomputing Institute for Digital Simulation and Advanced Computation's Basic Sciences Computing Laboratory. To date, the database has been used to compile data on suitable molecules for inclusion in a funding proposal.
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Alon V. McCormick, Fellow

Molecular Scale Chemical Reaction Engineering of Materials Synthesis

Molecular-scale models are being used in this research to characterize chemical engineering systems that pose special process modeling difficulties because they are governed by poorly understood molecular-scale interactions. To model the polymerization of silicon alkoxides and (meth)acrylates, these researchers are using Monte Carlo simulations to extract information about polymer size distribution, structure, and gelation. To perform computational chemistry calculations of silicate and (meth)acrylate energetics, they are using semi-empirical molecular orbital, molecular mechanics, molecular dynamics, and Monte Carlo packages. To study zeolite (and other molecular sieve) electronic structure, they perform ab initio electron density functional calculations and first principles molecular dynamics simulations.

Specific work is being done on zeolite formation at a molecular level. The researchers are using a hybrid two-scale computational approach. A pseudoclassical Monte Carlo method is used to model the interactions between silicate oligomers and structure-directing agents in water. This requires greater molecular detail, and molecular calculations are employed for this simulation. In the other approach, it is interesting to discriminate between layer-by-layer growth and agglomeration. This scenario can be amenable to meso-scale Monte Carlo simulations as it is typically employed in crystal growth modeling.

Other studies are being made on the behavior of molecules in nano-confined pores. Simulations are being used to study mobility of molecules, their adsorption dynamics, and separations. All of these may be different from what could be expected from bulk properties. These researchers have begun to look at aromaticsï¿½a set of molecules with complex geometryï¿½their packing behavior, mobility, and adsorption dynamics using Molecular Dynamics and Monte Carlo simulations. The overall study is putting forward a technique for economical separation of very like compounds with a high degree of purityï¿½something demanded by the pharmaceutical and speciality chemicals industry.

These projects begin to come together in looking at charge densities in zeolites. The researchers are focusing on the calculation of charge densities inside of zeolite pores. The research deals with first principles studies of zeolites utilizing a state-of-the-art first principles molecular dynamics with

variable cell shape. It self-consistently solves the electronic structure of the system at every time step of the dynamics to give an accurate representation of the interatomic bonding. This version of the molecular dynamics introduces strains in the simulations and removes all structural constraints.

A last piece of work being carried out by these researchers focuses on percolation simulations of crosslinking polymerization. It generally uses a two- or three-dimensional lattice with each site on the lattice representing a multifunctional monomer or initiator molecule. Radicals are generated with a certain initiation rate. At each time step, a neighbor of each radical is chosen. If the neighbor has not fully reacted, a chemical bond is formed and the radical function is transferred to this neighboring site. Thus, each of the radicals performs a nearly random walk on the lattice connecting a series of monomer units by chemical bonds. The walk of each radical continues until it meets another radical and both of them terminate or until it is trapped between fully reacted sites.

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David C. Morse, Principal Investigator

Computational Polymer Physics

These researchers are carrying out a program of Brownian dynamics simulations of the molecular dynamics and viscoelasticity of solutions of semi-flexible polymers. Among such polymers are a number of important biopolymers including DNA, collagen, cytoskeletal filaments such as actin, and most of the polymers that exhibit a nematic liquid-crystalline phase in solution such as Kevlar. Fluids of such worm-like chains are not describable by existing analytic theories of polymer dynamicsï¿½almost all of which treat polymers for simplicity as either completely flexible random walks or as completely rigid rods.

Recent work on the viscoelastic response of these solutions has clarified the different possible sources of stress in such solutions and has provided accurate analytic descriptions of the linear viscoelastic response in various asymtotic limits of high frequency, very strong entanglement, and very long or very short chain lengths. This work has successfully explained most features of the linear viscoelasticity of very highly entangled isotropic solutions of actin protein filaments, which have been intensively studied by biophysicists as models of the cellular cortex.

The Brownian dynamics simulations focus on simulations of the linear viscoelastic response of dilute solutions of worm-like chains. These simulations are based upon a well established algorithm for simulations of the Brownian motion of a model of a polymer as a series of links with constrained link

lengths, with bending forces between neighboring links. At each time step, deterministic forces arising from the bending energy and stochastic forces are first generated for each bead in the system, then Lagrange multiplier forces required to constrain all of the link lengths in the presence of these forces, and only then are the bead positions updated. The linear viscoelastic response of the solution is calculated by accumulating values of a temporal autocorrelation function of the mechanical stress, which is related to the time-dependent response to an imposed external strain by a theorem of statistical mechanics. The algorithm is inherently parallelizable since the main computational challenge will be to generate enough statistically independent stochastic histories to reduce the statistical error to manageable levels, which is most easily achieved by running many of completely independent simulations of non-interacting chains.

Further work is enlarging a program of computational statistical mechanics focusing on prediction of the structure and thermodynamics of ordered phases and structures of block copolymers. These calculations are based upon the self consistent mean field (SCMF) theory found to provide a remarkable quantitative description of copolymer microstructures. The mathematical operations required to calculate the structure and free energy for a periodic copolymer in the context of the polymer SCMF theory are essentially identical to those used to carry out a Hartree or local density approximation calculation for the electronic structure of a crystal.

Current focus is on SCMF calculations of the mechanical moduli of ordered copolymer microstructures, as measured in recent rheological experiments. Predictions for the moduli of ordered microstructures are obtained from calculations of the free energy in ordered phases with deformed unit cells. Preliminary calculations of this type have been carried out already. Simultaneous with work on calculating moduli, work is being done on the development of as modular, general, and efficient as possible a SCMF code for use in future work.

Research Group

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Two-Dimensional Reactor Modeling with Detailed Chemistry

The direct partial oxidation of alkanes (from methane to butane) at very short contact times has recently been shown to be a promising route to convert alkanes to more useful chemicals like syngas, olefins, and oxygenates. The processes are determined by an extremely fast variation of temperature, velocity, and transport coefficients of the reactive mixture at the catalyst entrance and involve a complex interaction of transport and kinetic effects. It is expected that modeling and simulation lead to a better understanding of these processes and accelerate scale-up to industrial operating conditions.

These researchers are using the computational fluid dynamics (CFD) code fluent to simulate the two-dimensional flow through a tubular catalytic reactor and over a wire gauze catalyst. The numerical results clearly show that detailed models for transport properties and chemistry have to be used to predict conversion and selectivity in these chemical reactors. While fluent is able to model transport processes in detail, there is a need of more sophisticated chemical models. Therefore, a new algorithm

calculating the surface and gas phase chemistry source terms in the governing equations is used, and newly developed subroutines were coupled to FLUENT. This procedure allows the researchers to study the influence of elementary reactions and surface coverage effects on global reactor selectivity and conversion. This numerical code has been applied to simulate direct partial oxidation of methane to syngas on nobel metal tubular catalysts.

Currently, these researchers are improving the solver to speed up its convergence behavior. The code is used for calculations of butane oxidation over catalytic wire gauzes. The studies of tubular systems is continued in parallel. Hereby, reactor conditions (composition, preheating, and pressure) is varied to find optimal conditions for industrial scale-up. Homogeneous gas phase reactions play an important role beside the catalytic surface reactions in these reactors at higher pressure. Therefore, the code is used for simulation of the reactor at higher pressure because this region cannot be studied safely or cost effectively in laboratory-scale experiments.

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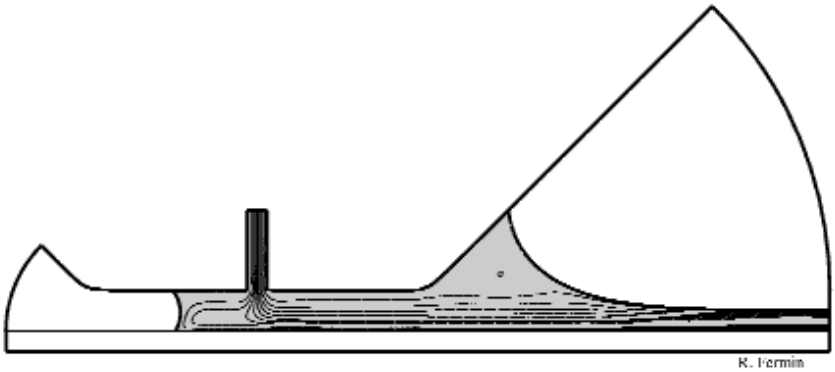
Physics of Fluids in Processing Technologies

This research is part of two large interrelated and coordinated research programs. One grew out of a program on the principles of enhanced oil recovery processes. The other grew out of a research program on the fluid mechanics on rheology of coating flows. Although this research is on fundamentals of liquid structures, flow, and transport, it is directed towards process technologies already commercially important or likely to become so. These include surfactancy, magnetic memory, high-speed printing and coating, high-performance polymers and plastics, deformation processing, chemical reaction processing (e.g., reaction injection molding, reaction coating, and sol-to-gel processing), drug delivery with fluid microstructures, solution mining, coal gasification, drying of multi-component and multilayer structures, and the similar technologies.

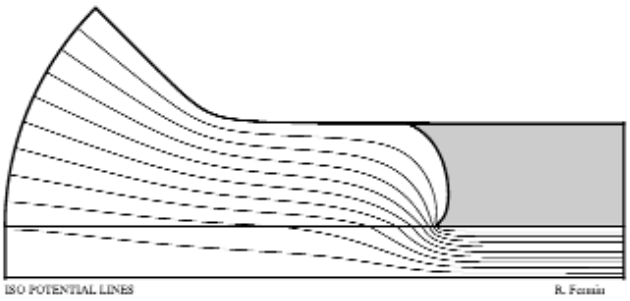
Problems are typically non-linear, multidimensional, often involve coupled partial differential and integral equations that describe simultaneous mass, energy, and momentum transport, and are frequently time dependent. Many problems involve free surfaces without constraining boundaries. The mathematical methods chiefly employed are those of subdomains, adaptive subdomaining, finite element basis functions, isoparametric mapping onto a computational domain, lumped-network modeling, Newton iteration with continuation, and adaptive time-stepping. To obtain information on the stability of solutions, the leading eigenvalues and corresponding eigenvectors are sought.

Usually, the structure of the solution spaceï¿½the number of solutions and their stability, folds, bifurcations, and so onï¿½is much more important than individual solutions. Many of the problems, though not excessively large, must be solved many times to map solution space, which requires large amounts of computer resources. The study of transient behavior typically demands two orders of magnitude more computational resources for a given problem. Three-dimensional problems and eigen problems of large systems have become accessible thanks to recent advances in microcomputer technology.

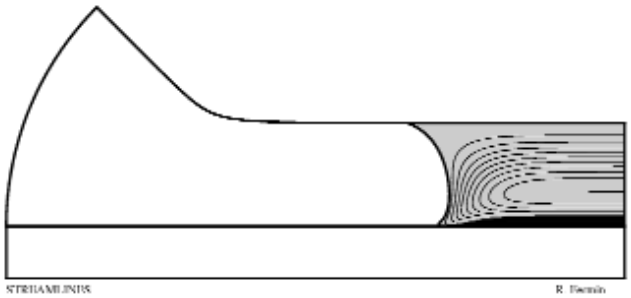
Because problems are solved repeatedly, efficient implementation of modern computer-aided mathematics is central to all research projects with emphasis on algorithms that take full advantage of computer capabilitiesï¿½namely parallelization and increasingly large memory and high-speed local memory. Of special interest to these researchers is parallelization of sparse matrix solvers (particularly frontal and iterative routines), implementation of mesh generation/adaptation strategies (especially those relying on solution of partial differential equations), optimization of generalized eigenproblem solvers (Arnoldi-type routines and others under development), efficient adaptation of iterative equation solvers (conjugate gradient and Arnoldi methods), especially adaptation of new software for preconditioned conjugate gradient and Generalized Minimum Residual (GMRES) methods, and utilization of sophisticated graphics and post-processors for interpretation and communication of the large amount of data produced by computer aided analysis.



Electrostatically assisted slot coating flow. An electric stress acts only at free surfaces in most practical coating flows. There, it is directed from the liquid phase to the gas phase. Properly deployed, this electric stress prevents or delays the onset of coating defects from wavy contact lines, contact line vees, air fingers, air entrainment, and coating bead breakup into rivulets.



Electrostatically assisted slot coating flow. Theoretical modeling of the electrostatically assisted slot coater continues. The Navier-Stokes system of equations in the liquid phase and a Laplace equation describing the static electric field in the gas and liquid phases are coupled at the air-liquid interface through interfacial boundary conditions. The coupled equations of base flows have been solved by the Galerkin/finite element method.



When the coating liquid is more conductive than the substrate, the resulting electric force on the upstream meniscus acts to collapse the entrained air film and pull the meniscus further upstream. The downstream meniscus is unaffected by the presence of the electric field. As the liquid-to-substrate conductivity ratio approaches unity, the electric force is no longer concentrated at the dynamic contact line but is distributed over the upstream meniscus.

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Matthew Tirrell, Principal

An Experimental and Simulation Study of Polymer Brushes in Steady and Oscillatory Shear Flow

The interfacial properties of a multiphase system can be dramatically altered by constraining polymers at the interface. When density of a polymer at the interface is high enough to cause neighboring chains to overlap, the polymer brush is formed. Polymer brushes have many technological applications including the stabilization of colloidal dispersions, enhanced lubrication between solid surfaces, and mixing of non-compatible homopolymers. In early scaling arguments, excluded volume interactions tending to stretch polymer chains away from the tethering surface were balanced by an entropic restoring force keeping them in a coil. The result was a brush with a uniform density of monomers and a scaling law for the height that varies linearly with N (the degree of polymerization of the tethered polymer) in a good solvent. Compared to the N3/5 scaling for the linear dimension of a free polymer in solution, considerable stretching can be seen by constraining a chain at one end. This simple theory of polymer brushes was further elaborated on by using a self-consistent field approach. Although the same brush height scaling was predicted as the earlier theories, the monomer density was found to vary parabolically within the brush.

While the equilibrium structures and properties of polymer brushes are well understood both theoretically and experimentally, the non-equilibrium situation is much less clear. Using the surface force apparatus (SFA), it was discovered that shearing two uncompressed brushes past one another can lead to an anomalous normal force pushing the brushes apart when the applied velocity is above critical threshold. Preliminary results of these researchers support this idea. They have particularly observed a "fanning out" of the tail of the SFA force profile. The dependence of this perturbation on the applied shear amplitude and frequency appears to differ between the molecular weight they have tested. Although some data exhibits many of the same qualitative features observed in the earlier experiments, subtle differences exist. Current theories usually attribute the appearance of additional normal force to a brush swelling effect. However, the cause of the swelling varies widely between different theories. Some credit hydrodynamic interactions between monomers while others suggest that chain stretching leads to increased excluded volume interactions between neighboring chains. Nevertheless, relatively few dynamic simulation studies have been done to shed some light on this subject.

Currently, both experiments and large-scale computer simulations are being used to study the behavior of polymer brushes under flow. Specifically, the SFA is used to investigate the range of frequencies and shear velocities at which there is an increase in normal force. Meanwhile, computer simulations using the technique of Brownian dynamics are being carried out within the same parameter range as in the experiments to provide a direct comparison and physical insights. Besides this brush swelling phenomenon, other interesting brush behavior is explored through large-scale simulations. The degree of interpenetration between two compressed brushes and the effect of solvent quality on brush dynamics and tribological properties are two such areas where simulations are helping to provide important insights into brush microstructures.

Research Group

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Robert T. Tranquillo, Associate Fellow

Stochastic Modeling of Receptor-Mediated Cell Motility

The first part of this project deals with the application and development of these researcherï¿½s anisotropic biphasic theory (ABT). The mechanical properties of acellular collagen gel are initially studied using the unconfined compression test (a cylindrical gel compressed between impermeable platens). Data from constant force (creep) and constant velocity (ramp) tests are fitted using the ABT in combination with the differential algebraic system solver with optimization (DASOPT) to obtain Poissonï¿½s ratio for collagen gel in conjunction with one-dimensional confined compression tests performed previously. A similar test to the creep test is being conducted with cells dispersed within the gel to study the effects of cell traction on collagen network reorganization, allowing cell traction and orientation parameters to be estimated. The finite element code for this isometric cell traction assay has already been developed so its incorporation into the code developed for the creep test should be straightforward.

The next step was aimed at developing a computer model to predict network behavior based on the structure of the network and the interaction between collagen fibrils. By developing such a model and applying it to the deformation of tissue-equivalents, the group should be able to greatly improve the accuracy and range of applicability of the ABT. This step is crucial to effective design of the bioartificial artery because of the large deformations involved in cell-induced compaction of a tube to form the bioartificial artery.

Currently, the group is in the process of applying the ABT equations to ocular biomechanics, particularly those related to glaucomaï¿½optic nerve damage generally associated with increased intraocular pressure. To better combat glaucoma, the group is developing a biomechanical model of the entire eye, accounting for the interaction between pure fluid, pure solid, and permeable gel. An additional question from ophthalmology is the mechanism by which the iris is pressed against the lens in some cases and the iris is pushed forward blocking the trabecular mesh in others. Both cases lead to increased intraocular pressure and glaucomatous damage to the optic nerve. The group is exploring this question numerically and experimentally by developing a model of the anterior portion of the eye to explore the interaction between aqueous humor flow and iris displacement.

The second part of the project deals with the stochastic model of receptor-mediated cytomechanics and chemotaxis. A model has already been formulated to explain the regulation of white blood cell locomotion in response to an external stimulus field. When the field is a spatial concentration gradient, this is the physiologically critical phenomenon known as chemotaxis. Using a continuum theory proposed to describe cytoplasmic forces and a stochastic description of the receptor signals generated on the cell surface, a stochastic partial differential equation (PDE) system has been formulated from which cell tracks can be simulated. Since this is essentially a problem of how a morphogenetic (pattern-forming) medium responds to external correlated noise, it is of fundamental importance. The current strategy involves using a combination of simulation (Cauchy-Euler method for the spatially-discretized system) and analytical or numerical methods (matrix methods to solve a linearization of the stochastic PDE system for correlation functions, providing a verification of simulation results as well as parametric dependence). Analysis of the first version of the model is currently complete, and a second version of the model is underway.

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First Principles Simulations of Materials under Pressure

These researchers interests revolve around the development and application of first principles molecular dynamics (FP-MD) algorithms. The technique used is an ab initio extended MD with variable cell shape. This reliable and predictive technique has made important predictions subjected to experimental verification in the past. Further development of this method and application to earth forming mineral phases under conditions typical of geological environments is currently funded by the National Science Foundation. The objective of this research is to provide a firm theoretical basis for a discussion of physics and chemistry of the earthï¿½s mantle.

Other problems of interest include pressure induced solid state amorphization, zeolite alumino-silicates, alumina and ruby, and more recently, magnetic oxides and first principles phonon thermodynamics.

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Jan Almlï¿½f, Principal Investigator *

Development and Application of Relativistic Methods for Heavy Metal Cluster Calculations

The Douglas-Kroll (DK) method is an electronic structure method suitable for including scalar relativistic effects in electronic structure calculations on large polyatomic systems. It employs a second order transformation of the Dirac-Coloumb relativistic Hamiltonian, which essentially decouples the large and small components of the wave function, and consequently reduces the complexity of four-component theory. Furthermore, the resulting two-component Hamiltonian is separable into spin-free and spin-dependent terms. The latter terms may be excluded in certain cases leading to a one-component spin-free ï¿½quasi-relativisticï¿½ Hamiltonian. This Hamiltonian, which contains non-singular operators, can be treated variationally and can be incorporated into standard programs for ab initio electronic structure calculations with minimal changes in the algorithms. This modified Hamiltonian is variationally stable, and it can be used in all types of electronic structure calculations (Hartree-Fock, Configuration Interaction, Mï¿½ller-Plesset perturbation theory, etc.). However, the integrals over these relativistic interactions are much too complicated to be evaluated analytically, and one must therefore use techniques involving spectral resolutions of the operators involved. These require large, uncontracted basis sets that lead to very resource-demanding transformations in the two-electron case.

These researchers are investigating two different approaches that utilize the intrinsic properties of the operators involved. These approaches use the hermitian property for the operators and two-electron operators. Treatment of the two-electron relativistic integrals with this scheme essentially simplifies the problem into modification and tracking of the contraction coefficients. Overall, using the one-component Douglas-Kroll method with the proposed schemes, relativistic calculations are done on an almost routine basis and open up a possible all electron study of heavy element chemistry including clusters. However, the inclusion of the spin-orbit term is far more complicated, and relatively few program systems including these terms are available. For these reasons, spin-dependent relativistic effects are mostly neglected, which is probably reasonable for ground state properties and highly coordinated compounds. However, such an approximation may not always be valid. For many compounds, including the third row transition metals, spin-orbit interactions are of the same order as the chemical binding. The DK spin-orbit terms are currently being included in the Hartree-Fock level in order to produce a two-component basis for already existing spin-orbit CI-programs.

* deceased, January 17, 1996

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Design and Characterization of Biomolecules: From Protein Core Modules to Cyclic Peptide Nucleic Acids

The engineering of stable, folded, and functional biomolecules has recently attracted a great deal of research attention. Within this field, these researchers are particularly interested in the design, synthesis, and characterization of protein core modules and cyclic peptide nucleic acids (PNAs).

In globular proteins, core motifs can be identified, and their elements can be combined in suitable peptides to construct native like modules. The designed peptides consist of core elements from Bovine Pancreatic Trypsin Inhibitor, a 58 residue protein with an array of three disulfide bonds, identified as the protein folding core on the basis of hydrogen isotope exchange, and B1 immuno-globulin binding domain of streptococcal protein G linked by natural or designed sequences, and a strategically placed crosslink to limit conformational space to more collapsed conformations. The ongoing and proposed studies exemplify new approaches and are leading to significant and generalizable insights that contribute to the protein folding problem.

Cyclic PNAs are promising candidates to generate nanotubular structures. Such nanotubular reagents can be useful as new catalysts, wire conductors, or drug transport systems. Cyclic PNAs are being designed by means of molecular modeling studies that assess the viability of cyclization as well as the molecular recognition mechanism between cyclic units.

Design and characterization studies in this field are computationally intensive. Fortunately, there is a great deal of useful software available. Once the designed molecules are synthesized, they are the subject of nuclear magnetic resonance spectroscopic studies from which structural features can be calculated.

Further work is being done on replacing disulfide cross-links with either the non-genetically encoded amino acid a-aminobutyric acid or alanine and then following the consequences by a battery of biophysical techniques. The results of these studies are also helping to provide insight into the protein folding problem.

Research Group

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Christopher J. Cramer, Fellow

Development and Application of Computational Chemistry for Purposes of Investigating Phenomena of Biological and Environmental Interest

This work is stressing the limit of current computational chemistry tools by use of supercomputer resources to examine large systems of relevance to areas in chemistry. In general, systems containing unpaired electrons, multiple metal atoms, or of a very large organic nature are being investigated.

The first area of focus is RNA dynamics. Nuclear magnetic resonance is a powerful technique for determining time-averaged structure of polynucleic acids. Measurements of internuclear nuclear Overhauser effects provides a set of distance constraints on various proton dyads. This information, used with a force-field minimization, generates a plausible nucleic acid structure. The researchers are now studying a structurally characterized alanine transfer-RNA using a tetraloop analog. The simulation includes a full environment and takes advantage of recent advances in simulation technology. Experimental data is used for a mutant version of the tetraloop known to have different properties with respect to charging the RNA with alanine.

The second project includes solvation effects in quantum chemical calculations. Early work has been successful in developing and calibrating models for any solvent at various theoretical levels. Current work involves the application of current solvation models to problems of chemical and biological interest and extension of the technology to more rigorous levels of theory. This project is developing new algorithms to calculate analytical gradients of the energy with respect to nuclear motion to more efficiently optimize molecular geometries.

The third focus of this research calculates accurate multiplet splittings in open-shell systems. Nitrenium ions are reactive intermediates implicated as carcinogenic products from aromatic amine catabolism. The divalent nitrenium ions covalently modify DNA in the carcinogenic event. Early theoretical work suggested arylnitrenium ions to be uniformly ground state singlets. Higher level calculations and experimental work done by this group has indicated that the triplet spin state may be preferred. This is critical since the mechanisms for reaction of the singlet compared to the triplet are distinct. Further work is comparing higher and lower levels of theory to determine how useful lower levels of theory are.

Another focus of the work is on understanding the structure and reactivity of phosphonothioate nerve agent VX with various nucleophiles. The researchers are studying reactions with hydroperoxide ions in aqueous solution to achieve a better understanding of the neutralization processes.

The last focus explores dicopper structures. The group is working to establish the spectroscopic properties of these molecules to make comparison with experiment and determine whether the molecules are well described as ground-state singlets with complete spin-pairing or whether symmetry breaking to localize one electron on each copper atom is advantageous. They are also working to more fully understand the effects of nature and location of counterions and the effects of solvation as well as

to gain a firm understanding of the molecular orbital issues that control relative stabilities of the two forms.

Professor Cramer is also teaching a class that is acquainting students with state-of-the-art hardware and software employed in modern molecular modeling. The students perform several experiments using the IBM SP and software packages including GAUSSIAN 94 and AMSOL.

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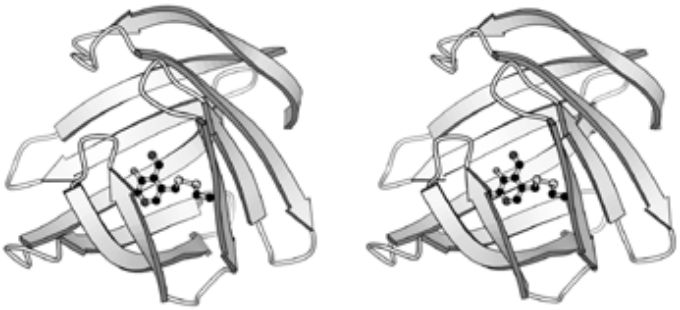
Design of Protein Catalysts

This work is developing enanatioselective catalysts that are based on protein cavities. This approach for catalyst design combines elements of host-guest chemistry with a highly flexible protein scaffold that can be manipulated by both chemical modification and recombinant DNA methods. The ability to prepare such catalysts could have a significant impact on the manufacture of a wide variety of specialty chemicals.

The researchers are improving the efficiency and controlling the specificity of transaminating catalysts based on protein cavities using site directed mutagenesis. They are assessing whether changes in cofactor structure can be used to modulate the properties of transaminating catalysts based on protein cavities. In addition, they are expanding the chemistry that can be performed using protein cavity based catalysts to include Carboni¿½Carbon bond formation. Overall, computer modeling is essential to accomplishing the goals of the project.



Model stereoview for the structure of a semisynthetic enzyme that catalyzes transamination reactions. This model is based on the structure of helixless IFABP solved by Cistola and coworkers.

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Craig J. Forsyth, Principal

Inhibition of Protein Phosphatases by Okadaic Acid and Related Natural Products

Protein phosphatases maintain proper levels of protein phosphorylation, and thus, they regulate a variety of important cellular processes including cell proliferation and protein synthesis. Protein phosphatases 1 and 2A (PP1 and PP2A) are inhibited by several natural products including okadaic acid and microcystin. Inhibition results in a number of important biological effects such as tumor

promotion. The crystal structure of PP1 co-crystallized with microcystin-LR is known, and it can be used to generate a model of PP1-microcystin.

These researchers are using insight software to build this model and create models of PP1 and PP2A with other inhibitors. These models are useful in studying potential binding contacts between inhibitor and protein and to identify important structural features required for inhibition. These modeling studies help support the larger research program by assisting in the design of inhibitors based on okadaic acid. These novel compounds are synthesized and tested in the laboratory.

Research Group

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Thomas R. Hoye, Principal

Design of Peptidomimetics as anti-HIV and Antiangiogenic Antitumor Agents

Molecular modeling is a powerful tool that guides the design of new targets for organic synthesis. Identification of novel, biologically active agents is one obviously valuable application. These researchers are designing non-peptidic analogs based on known, active, peptidic lead compounds. There are many projects where such approaches will benefit this research.

One example of such a project is the design of a class of enzyme inhibitors as potential anti-HIV agents. These are based upon structural information available from crystallographic studies of complexes between various peptidic agents (cyclosporin A and p55gag fragments) and human cyclophilin A. It is clear that the latter, host-cell protein must be recruited into new HIV virions to render the latter ineffective.

Another example of these projects is the design of new antiangiogenic antitumor agents. These are based upon knowledge of a requirement for certain side chain substituent nature and relative orientation in known antiangiogenic polypeptidic agents. Design of structures built on scaffolds that will display these residues in similar fashion are being guided by modeling studies.

Research Group

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Richard Hsung, Principal Investigator

Synthesis and Biological Evaluation of Arisugacin Analogs

This work is currently synthesizing CDE-ring analogs of a natural product (Arisugacin). The

researchers are using computational modeling to determine the active site where the analogs act on acetocholinesterase. Biological essays are utilized to test the efficiency of the analogs. The group is using insight and MACROMODEL to simulate the interaction between analogs and acetocholine esterase. They are rationalizing the key factors of these analogs responsible for the activity on the enzyme.

Research Group

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Steven Kass, Associate Fellow

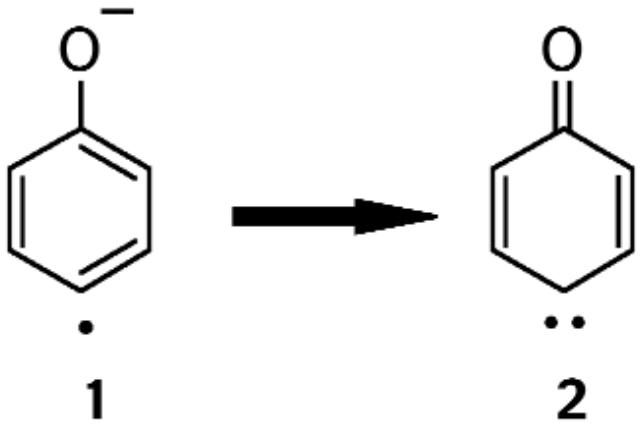
Understanding Organic Systems via Molecular Orbital Calculations

These researchers have recently developed a general method for the selective formation of radical anions in the gas phase. These species can serve as valuable precursors to a wide variety of reactive intermediates. A dicarboxylic acid is dissolved into a basic water-methanol or methanol-acetonitrile solution and dianions (or trianions) are sprayed into the gas phase with a Fourier transform mass spectrometer. Subsequent fragmentation via energetic collisions leads to radical anions. As anions and radical anions can be used to obtain quantitative thermodynamic information on the corresponding species with one less electron, the group is in a position to interrogate a whole treasure drove of transient (but highly important) molecules. For example, they have recently generated number 1 in the figure below and are in the process of measuring the stability (i.e., the heat of formation) of its corresponding carbene, number 2 below, an important species in photolithography. Consequently, they plan on carrying out ab initio and density functional theory (DFT) calculations on these and related species in order to obtain unique insights into these compounds; extensive calculations on some of the reactive intermediates are nearly complete.

Aromaticity and antiaromaticity are familiar and important concepts. Numerous examples of the former compounds have been reported, whereas the latter species have proven to be elusive and difficult to generate. The simplest member of the series and prototypical antiaromatic species, cyclopropenyl anion, has been considered as a possible substrate for the design of organic conducting polymers, but it had not been synthesized until this group described the first preparation of a cyclopropenyl anion. The group produced 3-carbomethoxycyclopropen-3-yl anion, a stable monosubstituted cyclopropenyl anion, at room temperature in their flowing afterglow device by reacting 3-carbomethoxy-(3-trimethylsilyl)cyclopropene with fluoride ion. They also used this approach to generate this ion as an intermediate in solution, and by modifying the substrate, the work is helping to lead in the formation of novel compounds with highly desirable properties. In order to gain a more detailed understanding of cyclopropenyl anion and its derivatives so that reasonable synthetic targets can be identified and prepared, high-level ab initio molecular orbital calculations have been carried out on a number of different species. Additional work needs to be carried out on compounds that hold the most promise for preparing a stable cyclopropenyl anion derivative.

Amino acids such as glycine exist in their zwitterionic form (+NH3CH2CO2-) in aqueous solutions over a wide pH range. In the gas phase, the neutral form (NH2CH2CO2H) dominates, but a few solvent molecules can selectively stabilize the zwitterion and have a profound impact on the potential energy

surface. Therefore, it stands to reason that many biological molecules exist as zwitterions in the gas phase. Very little is known about these species, and these researchers have started to investigate these from a computational point of view. They have already computed the potential energy surface on a relatively tractable zwitterionic ion and have started working on an experimentally more attractive but computationally more demanding system. It is more demanding because it is conformationally more flexible.



Measurements on 1 can provide the stability of 2 since the electron can be viewed as a "protecting group."

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Hung-wen Liu, Principal Investigator

Studies on the Inhibition of Enoyl COA-Hydratases by MCPF-COA

Enoyl COA-Hydratases (ECHs) are a family of enzymes involved in the second step of the b-oxidation pathway for long-chain fatty acids. These enzymes catalyze the stereo and regio-specific hydroxylation of aï¿½b unsaturated COA thioesters. This group has found that the compound MCPF-COA, which is the first inactivator to be discovered for these enzymes, shows different characteristics of inhibition with borine and rat ECHs. The current study involves a combination of homology modeling based on the X-ray structure of rat ECH, molecular modeling, and mutagenesis to explain the inhibition characteristics of MCPF-COA at the molecular level.

Research Group

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Timothy P. Lodge, Principal Investigator

Self-Consistent Calculations of Block Copolymer Solution Phase Behavior

Block copolymer systems have attracted considerable attention due to their ability to self-assemble into various ordered structures. These morphologies have novel material properties and valuable technological applications. Besides the importance to technology, the phase behavior of block copolymer systems is relevant to biological systems in which local segregation occurs and to surfactancy in general.

Research to date has focused on bulk copolymers. The mechanisms governing the self-assembly of AB block copolymer melts are well understood. The "classical" phases such as lamellae (L), hexagonal cylinders (C), body-centered cubic spheres (S), and more complicated phases such as the gyroid and hexagonally modulated and perforated layered phases have been examined both theoretically and experimentally. Although the phase behavior in melts is well established, it is difficult to achieve the microphase transition temperature with useful (i.e., high) molecular weights. Therefore, microphase-separated samples can be prepared from solution, where the unfavorable monomer-monomer interactions are partly screened. With the addition of a solvent into a block copolymer, phase behavior becomes more complicated due to the extra degrees of freedom provided by the solvent. When the solvent is neutral for both blocks, one anticipates similar phase transitions as in melts. In reality, most solvents are selective, and the solvent selectivity plays an important role in phase transitions of copolymer solutions. Recently, this group studied the distribution of nominally neutral and selective solvents in ordered block copolymer solutions. The study revealed that even a very slight degree of selectivity could lead to a measurable preferential swelling of one component. As more solvent is added, this effect of solvent preference is expected to be more significant. Besides solvent selectivity, the effects of other parameters such as concentration, temperature, composition, and molecular weight also need to be studied. Therefore, these researchers are mapping out the phase diagram of copolymer solutions systematically.

In this project, they are using the self-consistent mean-field (SCMF) theory to examine the phase behavior of block copolymers in the presence of a solvent. With the help of supercomputing resources, they developed a code and successfully applied it to construct the ï¿½classicalï¿½ phase diagrams. Recently, in the phase diagram calculations, this group included the more interesting complex phases such as the Gyroid (G) phase. The studies have shown that solvent selectivity and polymer concentration strongly influence the stability of the ordered microstructures. Upon the addition of a slightly selective solvent for the minority B blocks, a sequence of transitions from SB->CB->GB->L->GA->CA->SA->D (disordered) is possible. These numerical results have been observed in the experiments. In order to manifest this phenomenon, the group is examining the effect of solvent partition on interfacial tension and chain stretching energy in details. The competition between the two free energy terms has been examined to explain phase behavior in melts successfully. As the free energy balance is very delicate (and very controversial), many Fourier harmonics have to be included to compare the free energies.

Research Group

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Albert Moscowitz, Principal Investigator *

Molecular Geometries from Direct Inversion of Coulomb Explosion Imaging Data

It is experimentally possible to strip the valence shell electrons from atoms that comprise a molecule in times of the order of 10-16 seconds. The charged atomic centers thereby created all bear net charges of the same sign. Hence, those atomic centers will fly apart under coulombic forces (i.e., the molecule undergoes a so-called "coulomb explosion") and the positions and velocities of the particles arriving at a detector can be noted. This generated data can, in principle, be analyzed to provide information about the structure of the molecule at the time of the coulomb explosion. The method is sometimes referred to as the Coulomb Explosion Imaging (CEI) method. Computer simulations for the CEI experiments involve integration backward from the detector for the trajectories of each of the atomic ions generated as a result of a coulomb explosion. Current methods of analysis such as those currently employed at Argonne National Laboratory or the Weizmann Institute are limited to molecules of known or assumed symmetries. The University of Minnesota researchers have generated and are using a computer program that applies to molecules of unrestricted size and symmetry. Results obtained so far for model species give bond lengths and bond angles correct to one percent. The group is now applying the method to actual experimental data generated at Argonne National Laboratory and the Weizmann Institute.

* deceased, September 25, 1996

Research Group

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Eric Munson, Principal Investigator

Calculations of Nuclear Magnetic Resonance Chemical Shifts in Crystalline Organic Molecules

Understanding molecular conformations in crystalline organic compounds such as pharmaceuticals is important because drugs can exist in two or more crystalline phases that differ in arrangement and conformation of the molecules in the crystal lattice (polymorphism). The characterization of polymorphism is critical in the pharmaceutical sciences because different crystalline forms or polymorphs of the drug may display significant differences in solubility, bioavailability, processability, and physical/chemical stability. The existence of different polymorphs is easily determined from the solid-state nuclear magnetic resonance (NMR) spectrum. Despite the potential for using chemical shift in solid-state NMR spectra for structural determination in small organic molecules such as drugs, most studies to date only compare the NMR spectrum in the solid-state to the spectrum in solution.

Calculating NMR chemical shifts of crystalline organic compounds, such as drugs, relate experimental chemical shifts to molecular structure. Extensive work has been done on calculating chemical shifts in solution. In crystalline organic solids, the conformation of the molecule is already fixed. Theoretically, this would permit one step to be bypassed in the calculation, but the problem is that the NMR chemical shifts are very sensitive to the bond lengths, and the data obtained from single crystal X-ray diffraction data is not accurate enough to perform useful calculations. An energy minimization step must still be

incorporated, but the bond angles are fixed based upon the torsion angles determined from single crystal data, and the bond lengths will be optimized.

This group has two goals in calculating chemical shifts in crystalline solids. The first is to assist in the assignment of resonances in solid-state NMR spectra. This is a significant problem as peaks are often shifted by 10 ppm or more from their solution-state values, and there may be several peaks for each nucleus. Since many pharmaceutical compounds contain more than 10 carbon atoms and have solution-state chemical shifts within 10 ppm of each other, it is often impossible to assign all the resonances of interest by using the corresponding solution-state assignments. The initial strategy is to calculate the chemical shifts of the molecules using structural information provided by single crystal X-ray diffraction and see how well it correlates to the previously assigned chemical shifts obtained from solid-state NMR spectroscopy. The technique is then applied to systems that cannot be easily assigned, and calculated shifts are compared to peaks present in the NMR spectrum.

The second goal is to determine the crystal structure of a drug from the solid-state NMR spectrum. This strategy uses chemical shift calculations to predict torsion angles and bond distances for compounds based on the isotropic and anisotropic chemical shifts in the solid state. The researchers are not interested in accurately predicting the absolute chemical shift, but rather the chemical shift as a function of torsion angle. Once the approximate conformation or conformations of the molecule have been ascertained, they determine how the molecule packs into a crystalline lattice in its minimal energy configuration. They then refine the structure until the predicted powder X-ray diffraction pattern matches that of the experimentally observed pattern. By using a combination of procedures, this group is developing a robust method to determine the crystal structure of pharmaceutically-relevant solids for which no single-crystal data is available.

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Molecular Dynamics Simulations of transfer-RNA Acceptor Stem Variants

Recently, the nuclear magnetic resonance (NMR) structure of a 22-mer RNA hairpin loop that mimics the top part of the acceptor stem of transfer-RNAAla was reported. Experimentally, this group has shown that this small RNA is an excellent substrate for aminoacylation by alanine-transfer-RNA synthetase. However, a single G1:C18 to C1:G18 base pair transversion abolishes aminoacylation activity. Furthermore, substitution of the base pair analog C1:2-aminopurine (2AP) 18 restores considerable activity to the system. The only difference between the inactive C1:G18 hairpin and the active C1:2AP18 variant is that the latter lacks a 6-keto oxygen and N1 proton at position 18. The group has recently carried out 1.4 and 1.7 nanosecond simulations of the wild-type (G1:C18) and inactive C1:G18 hairpins beginning with the NMR structure. These simulations were accomplished by applying the particle mesh Ewald method with AMBER 4.1. They have compared the average

structures obtained from these simulations. They observed significant differences in the stacking interactions between the 1:18 base pairs and the adenosine at position 19 in the two structures. In particular, A19 appears to stack over the G present in the first base pair in each case. In the wild-type hairpin, this corresponds to intrastrand stacking with G1 while in the C1:G18 variant, this corresponds to intrastrand stacking with G18. These conformational differences may, in part, explain the different activities of the two RNAs. More recently, the group carried out a similar 1.5 nanosecond simulation with the C1:2AP18 variant. This study allowed them to correlate activity changes with changes in the conformation and stacking interactions around the 1:18 base pair and revealed new insights into transfer-RNA discrimination by aminoacyl-transfer-RNA synthetases.

In the C1:2-AP work, the simulation was performed using the average C1:G18 variant as a starting structure. To determine whether there is any bias in the outcome of the simulation, the group proposed to repeat the simulation starting with the average wild-type structure and building in the C1:2AP pair.

Research Group

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Jeffrey Roberts, Principal Investigator

A Theoretical Study of Diamond Growth Mechanisms and Morphology

These researchers are developing an atomistic understanding of morphology development during the chemical vapor deposition (CVD) of solid films. Solid films are typically composed of dense assemblies of nano- and microcrystalline particles. Morphology, in this situation, indicates average sizes, shapes, and relative orientations of the particles. In this work, the group seeks to understand why diamond CVD sometimes leads to crystallites that terminate in the 111-surface plane and other times, it leads to 100-terminated crystallites. More specifically, these researchers are investigating and quantifying differences between reactions that occur on, and produce, the 111 and 100 surfaces of diamond. Such information leads to a better understanding of the underlying mechanisms present in diamond growth, which in turn leads to differences in structure. This research increases the understanding of diamond growth. More specifically, it is at the very frontier of current efforts to model solid film growth.

Two types of methods are used in this project. The first involves ab initio calculations on small carbon/hydrogen clusters that model the diamond surface. Depending on the level of calculation, geometries and energies of molecules involved in important growth reactions can be calculated to a high degree of accuracy. The reactions critical to growth and morphology studied include hydrogen abstraction reactions from the diamond surface, methyl radical adsorption to the surface, hydrogen migration on the surface, and CH2 migration on the surface. Several hydrogen migration reactions and many abstraction and adsorption reactions have already been studied.

The current focus of this project is on CH2 migration reactions. The clusters of atoms are chosen so that they are large enough to represent bulk diamond but small enough to remain feasible computationally. Development and implementation of a program that simulates diamond growth is also

underway. A central objective of the simulations is prediction of morphology from parameters that can be experimentally controlled. The group believes that inclusion of surface migration reactions in simulations have a profound effect on morphology. This is due to relatively fast rates of carbon migration and energetic preference for carbon atoms to situate themselves in groups, or step edges, on the surface. The program runs by setting up an array of sites that represent sites on the diamond surface. Each site is then selected and tested for the occurrence of a reaction. The rates of reactions depend on environment surrounding the site in question. Energetics of the most critical reactions, including those discussed above, are calculated at ab initio levels. The probability of a reaction taking place depends upon reaction rates determined from reaction energetics combined with results found in literature. Simulations are performed that relate temperature and gas concentrations to resulting growth rates and film morphology.

Research Group

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J. Ilja Siepmann, Principal Investigator

Phase Equilibria of Complex Fluids: A Monte Carlo Study

Molecular modeling and other theoretical prediction methods are needed to complement available experimental data and improve rational design of efficient chemical processes. However, restrictions in theoretical techniques, force fields, and computational resources limit the range of systems to which molecular modeling can be successfully applied. These researchers are working to overcome these restrictions.

One focus for these researchers is on gas-liquid and reversed-phase liquid chromatographyï¿½the principal methods for analysis and separation of organic and pharmaceutical molecules. Work is being done to provide microscopic-level insight into chromatographic separation processes and to predict retention times using novel simulation techniques and transferable force fields. Configurational-bias Monte Carlo simulations in the Gibbs ensemble are employed to study the structures of stationary phases and to predict the partitioning of sample molecules between stationary liquid phase and mobile gas phase. In a first step, a stationary phase is modeled as a bulk liquid in thermodynamic contact with an interacting carrier gas. Three parameters are varied in the simulationsï¿½temperature, stationary phase composition, and solute. A diversity of solutes allows for a detailed investigation of the influence of shape, flexibility, and functionality on the retention process.

Other work is being done on free energies of transfer and phase equilibria for multicomponent mixtures. Configurational-bias Monte Carlo simulations in the Gibbs ensemble are being carried out to determine coexistence curves, critical points, and boiling points of some branched alkanes. These simulations help calculate the vapor-liquid coexistence loop for some binary systems and obtain the free energies of transfer for methanol, ethanol, and propanol between the solvents 1-octanol and water at standard conditions.

Further studies are being done on an all-atom model including interaction sites on the hydrogen atoms because it is intrinsically more realistic than the united-atom description that treats groups as pseudo-

atoms. United-atom models are more computationally tractable since they contain three times fewer interaction sites than atoms for a given hydrocarbon. The group has recently optimized their program by incorporating a molecule-based neighbor search before the calculation of site-site interactions. This should allow them to carry out calculations of the vapor-liquid phase envelopes for a series of linear and branched alkanes using all-atom potentials. To start, they tested five all-atom force fields. From simulations of vapor-liquid phase equilibria, they concluded that none of the force fields perform satisfactorily in predictions of thermodynamic properties. Thus, they are deriving a new parameterization.

Another study is being done on phase equilibria of multi-component systems containing at least one component in its supercritical state. The simulations provide detailed molecular-level insight as to how supercritical fluids dissolve solutes and why the addition of small quantities of an entrainer can greatly increase solubility power. The group suggested three systems of increasing complexity for a detailed studyï¿½a binary mixture of two linear alkanes, the solvation of n-hexane and n-octacosane in supercritical carbon dioxide, and a ternary system consisting of the supercritical fluid (ethane), a co-solvent, and the solute.

The last area this group is working on is developing algorithmic advances for the Monte Carlo simulations. They are working toward developing more efficient ways to sample the configuration space of molecules and reduce the expense of utilizing polarizable force fields.

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Computational Chemical Dynamics

These researchers are continuing their study of electronically nonadiabatic processes in the NaH2 system (which has a conical intersection) and the NaHF system (which has an avoided crossing). They are also performing calculations on model potential energy surfaces with customizable features. Quantal calculations on these systems help to provide insight into the relationship between features on the potential energy surface and dynamical properties of photochemical systems. Another project involves quantum dynamics studies on the Cl-H2 system and its deuterated analog. They are calculating differential cross sections for the Cl + D2 reaction and comparing the results to quasiclassical studies and experiments.

The groupï¿½s computer program POLYRATE uses variational transition state theory and multidimensional semiclassical tunneling contributions to calculate reaction rates for polyatomic systems. They are developing new methods and interfaces that increase the efficiency of computing reaction rates and the accuracy of the computed reaction rates. They are reaction rates of large biological systems as well as organic chemical reaction rates in the condensed phase. In order to fully utilize the power of multi-processor computing, they are extending development of POLYRATE to multi-processor platforms. The parallelization strategy involves rearrangement of the algorithm so that the reaction path is calculated first and the Hessians are calculated in parallel.

The key step in many enzymatic reactions is a hydride transfer that is accelerated by tunneling. The influence of the solvent is extremely important in affecting not only the transfer process, but also the conformation of the enzymes that catalyze these kind of reactions. In this project, the group is modeling hydride transfer in enzymes using POLYRATE and other tools previously developed in the group, particularly the equilibrium solution approximation, dual-level dynamics, dual-level electronic structure calculation, and multiconfiguration molecular mechanics.

The group is also simulating the photodissociation of the vibrationally excited quasi-bound states of the HF dimer by fully converged four-body quantum dynamics because reduced-dimensionality calculations do not agree with experiment.

The group has parameterized tight-binding theory for systems consisting of Ni, C, and H. With these parameters, dynamical calculations are now underway. The researchers are extending the study to systems consisting of Cu, Pd, Ag, Pt, and Au interacting with hydrocarbons. They perform the parameterization using genetic algorithms and target points of the potential energy surfaces which are calculated using GAUSSIAN-94.

The pairing of ions in solution plays an important role in many biological and industrial problems and in applications such as macromolecular association and catalysis. The SMx models have been shown to be highly successful at predicting solvation free energies of individual solutes in a diverse collection of solvents. The group is using the models to calculate the interactions of ion pairs and neutral pairs in solution. Since the existing models were not parameterized to capture these multiple-body interactions, a new model is under development.

The group has also begun to implement analytical gradients for the solvation models based on CM2 atomic charges. The group has derived the formulae for the analytical energy gradients in their self-consistent reaction field solvation model. They are currently constructing a module to implement these formulae.

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Xiaoyang Zhu, Principal Investigator

Wavepacket Simulation of Surface Dynamic Processes

Chemical kinetics on semiconductor surfaces is of immense importance. From an applied perspective, one of the most important processes for the growth of semiconductor thin films is chemical vapor deposition (CVD), and surface reaction kinetics is increasingly becoming a dominant factor in CVD due to the ever more stringent demand on spatial and chemical control. Despite intense interest in CVD surface kinetics, most studies fall short of addressing the molecular basis. From a physical chemistry perspective, reaction dynamics on semiconductor surfaces differ fundamentally from those in the gas phase; the presence of the surface introduces a host of new energy transfer pathways. In addition, semiconductor surface dynamics also differ from corresponding processes on metal. On metal surfaces the dominant energy transfer pathway is the excitation of electron-hole pairs in the substrate. This energy transfer pathway is absent on semiconductor surfaces. From a computational point of view, semiconductor surfaces are also more attractive than metals. The covalent and localized nature of bonding on semiconductor surfaces may allow high level calculations using a relatively small cluster to simulate the real surface.

In view of these interests, these researchers are unveiling the fundamental surface reaction dynamics in model semiconductor systems. Experiments underway are aimed at establishing the quantum-state resolved distributions of nascent gas-phase products from semiconductor surface reactions; the photodesorption of hydrogen from Si(100), H - Si + hn -> H (g) + _Si; and the abstraction of surface hydrogen on Si(100) by atomic H, H + H - Si -> H2 (g) + _Si. Here, _ denotes a surface dangling bond. The first reaction is an example for nonthermal dynamics on surfaces and the second is similar to many well characterized gas phase processesï¿½A + BC -> AB + C. Both reactions are not only ideal model

systems but also of immense technological interests. The energetic information carried by gas-phase "messengers" may be used to address fundamental questions. To answer these questions, this research group is carrying out time-dependent quantum mechanical simulations on ab initio potential energy surfaces and comparing computational results with experimental measurements.

The computational method is based on solving the time-dependent Schrodinger equation in discrete phase space using the Fast-Fourier-Transform (FFT) method. The computer codes have already been developed in the laboratory. Preliminary calculations for the photodesorption of H from Si(100) has relvealed the ultrafast dynamic process represented by a three step process; the initial excitation moves the system to an electronically excited potential energy surface (PES). Following excitation, the nuclear wavefunction propagates on the excited PES. While in the gas phase, this nuclear movement may lead exclusively to dissociation. The efficient quenching process on a semiconductor surface is fastï¿½on the order of 10-15s, shorter than the time required for the complete separation of the dissociating bond. As a result, electronic quenching brings the system back down to the ground PES after certain lifetime. The non-stationary wavefunction then propagates on a longer time scale on the ground PES. The wavepacket in the asymptotic region corresponds to desorption. This simulation yields important experimental observables including desorption quantum yield, isotope effect, and product (H) translational distribution. Computer codes for multidimensional wavepacket simulations are currently under development.

Research Group

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Robert Dexter, Principal Investigator

Effect of Welded Stiffeners on Crack Growth

The advent of high strength steel allowed engineers to design using more compact shapes at higher stresses. Oil tankers in the Trans Alaskan Pipeline Service (TAPS) trade were one of the first structures to utilize the stronger steel. In designing for higher stresses, the incidence of fatigue cracking has increased tremendously in ship hulls. This is because fatigue crack growth is directly proportional to applied stress range, andï¿½while the yield strength of high strength steel may be largerï¿½fracture

toughness of the high strength steel is not increased. In fracture mechanics, this translates to a higher incidence of cracking.

At present, TAPS trade oil tankers are required to routinely inspect for cracks. Any cracks found must be documented, and an estimated time to a critical crack length must be calculated. Such calculations are currently based on brittle material behavior and are far too conservative for the ductile materials these ships consist of. In many cases, cracks have been observed to grow in a stable manner at lengths one hundred times greater than the current formulations suggest is possible.

The current proposal is funded by the United States Coast Guard to better define crack propagation behavior in structures that incorporate welded, stiffened panelsï¿½namely the TAPS trade tankers or similar vessels. An analytical model and finite element model is being created and calibrated with full scale experimental testing, allowing calculation of a worst case crack growth scenario. The finite element program ABAQUS, whose employment is an essential part of models refined for use in the shipping industry, is being used to model the crack growth in a three-dimensional environment incorporating the effects of residual stresses induced by welded stiffeners. Residual stresses have been shown to be a key parameter in the rate of crack growth, and finite element analysis has proven to be an effective modeling tool for this situation in earlier research.

ABAQUS is used to calculate the J-integral around a crack tip for many instances of crack growth and geometry. This J-integral is directly utilized in an estimation of crack propagation rate at discrete increments in crack length. The methodology has been well established and used in previous research to generate good correlation with observed crack growth rates. Furthermore, the use of a finite element model proves to be an effective visualization tool for observing residual stress field changes in response to crack growth, the effects of load shedding due to severed stiffeners, and changes in the overall stress field surrounding a growing crack. Such a visual aid allows easier recognition of unforeseen factors in predicting fatigue crack growth.

Research Group

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Catherine W. French, Principal Investigator and Carol Shield, Co-Principal Investigator

Pre-release Cracks in Prestressed Girders

This project is investigating the effect of pre-release cracks on prestressed concrete bridge girders. Before prestressed bridge girder strands are released from the pretensioning bed, some bridge girders have been observed to incur vertical cracks that extend from the top flange toward the bottom flange in the girder cross section. These cracks are suspected to cause a reduction in the camber and in the loads to initiate flexural cracking in the bottom fiber of the girder. A geometric compatibility theory was developed to explain this behavior. This work is attempting to validate this theory with numerical results from abaqus. Analyses are used to learn the extent of camber reduction and what localized

effects these cracks have on prestressed girders.

Significant progress has been made towards discovering the effect of prerelease cracks on prestressed concrete bridge girders. Several crack depths have been analyzed, and it has been determined that the effect of prerelease cracks is a local effect. The action of the beam to close the crack causes a reduction in the camber of the girder. The ABAQUS results compare well with the geometric compatibility theory already described. However, there is a behavior that is occurring in the girders that disagrees with the geometric compatibility theory. This behavior is currently under investigation. The geometric theory is based on the crack closing by pivoting about the tip of the crack. This would mean that the greatest bottom fiber stress effect for a given crack width would occur when the prerelease crack is very shallow. This effect would then have a linear decrease in the stress effect with cracks of greater depth. This is not the case when the ABAQUS results are examined. There appears to be a critical depth of crack that causes the greatest bottom fiber stress effect. This critical crack depth is currently being determined. A model of a girder that was cast and tested is also being analyzed. These results will then be compared to the empirical data collected when the girder was tested.

Research Group

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Bojan Guzina, Principal Investigator

Numerical Solutions in Geotechnical Subsurface Sensing

A key component in the design process in civil engineering is geotechnical site exploration. Owing to the limited resources allotted to exploration programs and the natural variability of soil profiles, much of the information about the site is reliant on engineering judgment and interpolation of data available from discrete sampling of soil deposits. In recognition of such limitations, the last decade has witnessed significant advances in dynamic site characterization as a means to continuously probe large volumes of soils. Among such methods, the non-invasive seismic techniques represent a particularly efficient complement to standard exploration programs. In view of the complexity of underlying wave propagation problems, the seismic methods are typically based on approximate theoretical models that use wave velocity measurements as an input. These deficiencies, among others, can lead to multiple interpretations of experimental data resulting in non-unique estimates of subsurface profiles.

The central theme of the work is on development of a novel method for non-intrusive testing of horizontally-stratified subsurface profiles. The technique is based on the full waveform analysis of the ground surface motion and provides information about the stiffness, density, and damping properties of the profile tested. Analyses employ the rigorous three-dimensional wave propagation solution for a multi-layered viscoelastic medium. The forward model is effectively coupled with an appropriate inversion algorithm. In the work, material properties of the layered medium are inverted by systematically adjusting the initial model parameters according to discrepancies between the measured and predicted records of surface displacements generated by a dynamic source. The method revolves around the theory of inverse methods for a linearized system where differences between observed and calculated data are related to the parameter perturbations of the initial model through a system of linear

algebraic equations. Recognizing the fact that motion in a stratified medium is a non-linear function of the layer parameters and allowing for the possibility that the assumed initial profile significantly differs from the actual site stratigraphy, selected linearized inversion methods are employed in an iterative fashion. Final choice of the inversion algorithmï¿½such as the generalized inverse, the maximum-likelihood inverse, the stochastic inverse, or the damped least-squares solutionï¿½will be based on efficiency and convergence of the method in context to the problem examined. Issues such as uniqueness, resolution, and error of the solution are being investigated. To allow the a priori information about the site tested to be effectively incorporated into the characterization process, inequality constraints to the inversion method are also being considered.

The prototype inversion algorithm for uniform subsurface profiles, based on the full waveform analysis and the maximum likelihood inverse, has already been developed and tested. Apart from serving as an effective tool for site and material characterization in terms of their equivalent-uniform material properties, the analysis developed furnishes a rational basis for the extensions of the methodology to more general multi-layered models.

Research Group

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Computational Simulation of Ultrasonic Damage Assessment in Concrete Materials

The objective of this project is to determine the change of material properties with the aid of ultrasonic wave transmission techniques when concrete specimens are subjected to stress induced damage.

The project includes experimental, computational, and theoretical research. Specific developments include ultrasonic experiments on concrete specimens loaded under cyclic compression, numerical simulation of ultrasonic wave transmission, and characterization of progressive damage including separation of elastic stiffness degradation from inelastic dissipation.

Significant computational resources are required for the numerical simulation of the ultrasonic experiments. Initial computational efforts at the University of Colorado at Boulder involved wave propagation studies in linear elastic and elastoplastic two-dimensional domains. The current proposal is a continuation of these initial computational studies with three objectives in mind. The first is to expand the two-dimensional ultrasonic simulations with additional sensitivity studies. The second is to extend the computations to three-dimensional domains in space and time. The last is to examine dispersion effects of the heterogeneous microstructure for quantifying attenuation measurements. This long term objective on dispersion in concrete materials is of particular challenge because of the numerical dispersion effects due to finite element meshing.

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Microcrack Characterization of Failure in Rock-like Materials

Acoustic emission (AE), the sudden release of strain energy from microcracks in rock, is a technique that can be used to analyze the development of failure in rock-like materials. The recorded signals contain information about the source eventï¿½location and type.

Quantitative characterization of acoustic emission is concerned with the determination of the type of source mechanism. In the analysis, each microseismic event is idealized as a point source of displacement discontinuity, which can be modeled as a combination of couples of body forces that yield the same elastic wave field as the defect. Because of the difficulties involved in the visual observation of actual acoustic emission sources, numerical modeling becomes a very useful tool in verifying the predictions of AE source modeling.

This research is based on the use of a boundary elements code to model and reproduce the results from laboratory tests of rock fracturing. The material is represented by a mesh of displacement discontinuity elements that constitutes potential new surfaces of an incremental crack growth process. The process of rock fracturing is simulated by performing a search routine on all displacement discontinuity elements for each loading step. Displacement is then allowed on all elements that satisfy a chosen failure criterion, one element at a time, by selecting the element that corresponds to the largest unbalanced force for each iteration. A very large amount of memory is required in order to have a realistic representation of this microcrack associated failure process, which requires displacement discontinuity elements that are approximately of the same order of magnitude as the grain size of the material. The results obtained so far have shown very good agreement with laboratory results from a uniaxial compression test, both in terms of effective properties and strength. Additional work includes an attempt to verify measurements of energy release from acoustic emission techniques.

These researchers are also looking into damage mechanisms around a circular opening under biaxial compression. A study of a circular tunnel subjected to a biaxial state of stresses is modeled in the laboratory by a prismatic specimen of Berea sandstone under plane strain compression. The progressive failure is monitored using an AE system with eight piezoelectric sensors placed on lateral surfaces of the specimen. In addition, numerical analysis is used to detect fracture propagation in this problem.

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An Analysis of the Constituitive Models for Pavement Response

The Minnesota Road Research Facility (Mn/ROAD) is one of the most advanced road research facilities in the world. This facility includes six miles of roadway consisting of over forty different pavement designs. One segment of the roadway carries live interstate traffic. Over 4,800 temperature, moisture, frost, deflection, and static and dynamic strain sensors have been embedded in these test sections.

Like any structure, the performance of a pavement is dependent on the properties of the materials used to construct the pavement and how these are arranged to form a structure. To optimize design, the engineer must determine what material properties and design parameters contribute to good performance.

The forty pavement designs at Mn/ROAD are representative of the types of pavements currently being constructed throughout the state of Minnesota. This provides an opportunity to measure the response of a pavement to an applied load under known environmental conditions. This field data has been collected and is now calibrating models of the pavement sections so the influence of characteristics can be further defined for a larger range of variables.

Falling weight deflectometers (FWD) are commonly used devices for performing structural evaluations on pavement. FWD testing consists of dropping a weight packet on the pavement and recording the resulting deflections at various distances. The known weight and measured deflections can be used to locate voids under the slab, backcalculate the material properties of each pavement layer, or to monitor the performance of the joint and cracks in the slab. The purpose of this project is to provide a method for analyzing FWD data that would allow engineers to account for the non-uniform support conditions under the slab due to the presence of a temperature or moisture gradient. Currently, the presence of a temperature or moisture gradient is not considered. The ability of a joint or crack to transfer a load from one side of the discontinuity to the other, the backcalculated material properties, or support conditions under the slab can be either over or under estimated depending on the gradient present.

A two-phase approach was taken to quantify the effects of the gradients on the resulting deflections. The first portion of this project included a major data collection effort at the Mn/ROAD research site. Temperature, moisture, static and dynamic strain, and profile measurements were recorded in

conjunction with FWD testing at various times of the year throughout a twenty-four hour period. This data is now being used to calibrate three-dimensional finite element models using the abaqus finite element package so that additional response data can be generated for a larger range of parameters. The finite element generated data is combined with the field data to develop models that assist engineers when analyzing FWD data for pavements with temperature/moisture gradients.

One of the Mn/ROAD projects is to develop a mechanistic-based design method. The method is based on the mechanical response of a pavement structure, such as stress, strain, and deflection. The calculation of the pavement response greatly depends on constitutive models of materials composed of the pavement structure. For instance, subgrade and base materials can be modeled as a linear elastic or plastic material. In order to study the influence of different constitutive models on pavement response, a numerical calculation is necessary. Calculated results are then compared with Mn/ROAD in-situ pavement data to verify the theoretical models.

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Analysis of Stress Fields in Drying Viscoelastic Materials

Drying and cooling accompanies many industrial processes such as photographic, magnetic, or protective coating, injection molding, and curing of concrete structures. This is always associated with volumetric changes, sometimes very large, and with changes in material properties. Such changes are typically nonuniform in space and are often incompatible with the conditions imposed by the surrounding material. As a result, stresses almost always develop in drying or cooling materials, and various defects of the manufactured product may occur. Predicting these stresses and controlling their magnitude is an important goal with various potential applications.

In this project, a model is being developed to describe development of stress and deformation fields in drying viscoelastic materials. Materials with the properties are frequently used in practice. The model is based on large deformation theory, referring to multiplicative decomposition of the deformation gradient into its elastic and viscous part. The third part, representing volumetric changes of the material, is added in a similar, multiplicative fashion and is connected through the appropriate constitutive equations to the variables representing current state of drying or cooling. These variables are governed by diffusion-type equations written for the medium that moves as a result of large deformations. Together, all this leads to a highly nonlinear system and constitutes one academic side of this project.

The second academic side of the project includes the development of a numerical technique to solve the resulting system of nonlinear equations and its computer implementation. In this process, the equations are discretized using the finite element method. The resulting semidiscrete system of equations are integrated in time numerically and consistently linearized to solve the problem incrementally.

Stability of Pile Groups

Bridge scour is a serious practical problem that may lead to structural failure. Recognizing this, relevant transportation authorities mandated analysis of the effects scour may have on the stability (integrity) of the bridge structure. The goal of this project is to determine a depth to which scour can be tolerated. Furthermore, work is being done to discover whether this depth is related to type of soil in the area, number of piles, and nature of interaction between them.

From the theoretical point of view, the problem is complex for a variety of reasons. First, to examine stability and postbuckling behavior of structures, one has to consider the problem within fully nonlinear theory; large rotations and large displacements have to be considered. Second, interaction with soil adds immensely to the complexity in view of the fact that soils are materials with inherently nonlinear behavior. Third, since the parameters such as critical (maximum allowed) depth of scour has to be determined in the process, either a big number of independent calculations has to be made or some sort of (nonlinear) optimization techniques have to be used.

A theory that could be used to handle the structural part of the model has been developed. The theory is fairly established. A less established and demanding further development is the part having to do with the soil-structure interaction problem. In the past, this has been modeled as elastic interaction. While in the analysis not involving critical state, such as buckling, this assumption can be quite satisfactory, it is anticipated that this may not be the case in the analysis of buckling. That hypothesis is being verified in the current research.

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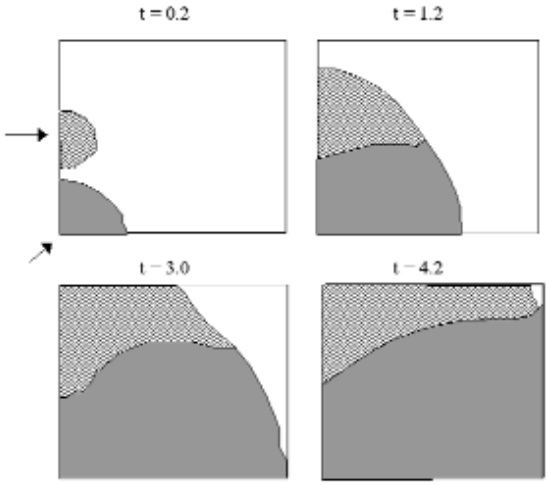
Numerical Solutions of Free and Moving Boundary Problems

Many industrial and natural processes involve the transport of conserved quantities. Typically, modeling of these processes involves the solution of partial differential equations in domains with well-defined boundaries. However, there is a wide class of problems that involve free or moving boundaries. In these problems, the location of one or more domain boundary is an unknown in the problem (a free boundary) or a boundary on which balance conditions have to be met as it moves through the domain. The classical example is tracking of the solid/liquid interface during melting of ice.

Early work in this project focused on developing computational tools for the analysis of free surface and moving boundary problems encountered in solidification processes. The aim of current work is to extend investigations to more general problems in diverse areas extending from materials processing to geology.

One specific area of interest is product and process engineering for starch based polymers. In this area,

an engineering methodology is being created to routinely design products using environmentally friendly starch-based polymers. The current focus of work is in the development of numerical tools for modeling.



The figure shows numerical filling predictions (in plain view) of the injection of two dissimilar polymers into a thin (initially empty) mold from constant pressure sources. There are two free boundaries in this problem. The first is between the polymer and the air in the empty mold, and the second is between the two polymers. These solutions were obtained with a fixed finite volume grid calculation that used a mixture of Volume of Fluid (VOF) and Level Set Methods.

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Aspects of Unsteady Sheet/Cloud Cavitation

The science of cavitation has evolved into a phase where detailed dynamics of unsteady processes are of prime concern. An important goal for cavitation research is the development of numerical models that can accurately predict the cavitation behavior in a variety of applications where cavitation is unavoidable. Examples of this are marine propellers, pumps, and hydroturbines.

The scope of the current project on unsteady sheet-cavitation is to experimentally identify the physics of the non-stationary processes. This information is impacting future numerical modeling in this phenomena. By developing a numerical model in concert with experimentation to describe the complex physics, the goal of obtaining reliable predictive tools is ensured.

Because the physics of the problem is highly complex and unsteady, it is essential that the entire experimental system is modeled to ensure that observed phenomena are simply an artifact of the experimental setup. Therefore, it is necessary to numerically model the water tunnel used for experimentation in order to relate any observed phenomena to the specifics of the tunnel.

This problem is fairly large and uses fluent to aid in the modeling. Further efforts are being made with the fluent program to exploit its capabilities on calculating two phase flows. The ability to use the added features in fluent help the total project develop new techniques for the measurement of cavitation flows.

Finally, efforts are being made to collaborate with other researchers at the St. Anthony Falls Laboratory. This serves as validation for the cavitation modeling and for modeling of the effects this research group observes in the water tunnel. In addition to working with Fluent, these researchers are in close collaboration with Professor Charles C.S. Song and Dr. Jianming He. Together, they have made careful measurements in the wake of a hydrofoil with and without cavitation. The work using fluent predicts the non-cavitating wake well. Professor Songï¿½s large eddy simulation (LES) model does a good job of predicting the wake under cavitating conditions. Results of this work can be seen in the figures on the previous page.

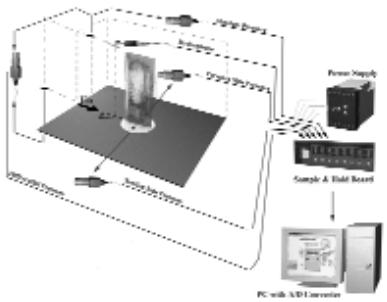

Figure 1: Test Setup

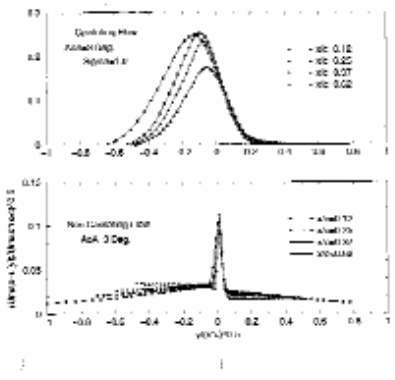

Figure 2: Measured Data

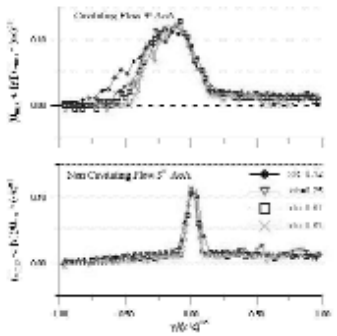

Figure 3: Simulations using a large eddy simulation (LES) model.

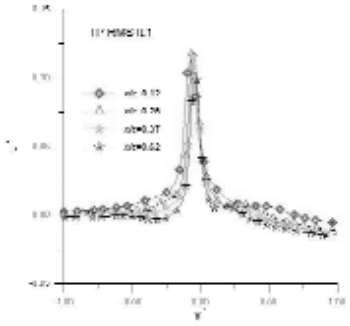

Figure 4: Simulations using fluent 5 with a Reynolds Stress Model

Comparisons are made between measured experimental data and simulations for the wake of a hydrofoil. Measurements were made in a water tunnel at various distances behind the trailing edge of a hydrofoil as shown in Figure 1. The data are plotted in the form [Umax ï¿½ u(y)]/Umax *(x/c)0.5 versus y/(x*c)0.5 where Umax is the free stream velocity, c is chord length, u(y) is the axial component of velocity in the wake, y is normal to the flow with negative values on the suction side of the foil, and x is the distance downstream of the trailing edge of the foil. Comparisons are made with the large eddy simulations (LES) of Song and He and these researchers simulations using an RSM model in FLUENT 5.

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Numerical and Physical Modeling of Wind Tunnel Flows

This project was dealing with the simulation of atmospheric boundary layers and the development of data acquisition and software capabilities necessary to carry out the intended measurements. Presently, the focus is on statistical processing of the vast amount of data sets being generated by the boundary layer and bluff body flow measurements currently underway. In addition to the data processing needs, the purpose of the research is to develop and test computer programs to model the flow in wind tunnel components, specifically closed circuit tunnel contractions and indraft inlets for open circuit tunnels, and to develop and test codes to calculate flows about bluff bodies.

Euler equations for nearly incompressible flow have been solved for two-dimensional, axisymmetric, and three-dimensional (specifically square-to-square and square-to-rectangular) contractions using an explicit finite volume scheme. The method obtains the steady state solution of interest as the limit for infinite time of the unsteady solution to a system of hyperbolic equations with arbitrarily imposed initial conditions. The Euler code does not require the assumption of irrotational flow and affords more

realistic flow simulations than irrotational flow codes. Furthermore, it provides a calculational scheme for certain unsteady flow problems of interest that require both unsteady and rotational flow computations.

While generation of the grid in the two-dimensional, axisymmetric, and three-dimensional cases proved to be a relatively straightforward task, the treatment of the boundary conditions was more involved. The nearly incompressible flow assumption has proven to be more efficient than any direct solution of the steady rotational flow equations so far. Further improvements of the code efficiency have come from the use of vectorization capabilities and from the use of certain types of boundary conditions suggested by physical considerations to shorten the time required for convergence of the wave-like oscillations that characterize the unsteady solution.

The latter technique has been successfully implemented for both steady rotational and irrotational flow through a contraction. By imposing a time-varying pressure boundary condition, the pressure waves produced by the method are effectively damped out, and the computing time necessary to achieve the steady state solution becomes an order of magnitude smaller.

For the particular problem of boundary layer development and possible occurrence of relaminarization, a combined experimental-numerical approach was used. To predict the boundary layer velocity profiles when relaminarization occurs, a two-equation turbulence closure model was applied in the calculations. The overall computational model includes the equation of continuity, the Reynolds equation, and the transport equations for turbulence kinetic energy and kinetic energy dissipation. The distribution of turbulent viscosity in the flow was obtained by solving for these two transport equations. The calculation domain was divided into near-wall and far-wall regions. Low- and high-turbulence-Reynolds-number forms of the turbulence models were respectively applied. The numerical results were in good agreement with data taken in a wind tunnel facility. Further applications of this code and comparison with experimental data are still needed and are currently being worked on.

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Space-Time Precipitation Variability and Predictability

Accurate forecasting of the onset, duration, locality, intensity, and type of precipitation is one of the most difficult challenges facing modern-day meteorology. It has become clear that the next quantum leap in Quantitative Precipitation Forecasting (QPF) will arise from explicit representation of storm-scale features in non-hydrostatic numerical models. While challenges associated with this are broad and significant, three interrelated aspects are of considerable importance and are being addressed in this groupï¿½s work.

First, the storm-scale QPF problem itself is an extreme challenge. An initial step involves establishing and correcting deficiencies in current microphysical parameterization schemes. Procedures for effectively using data are already well explored and results are encouraging. However, methods comparing forecasted high-resolution precipitation patterns to observed ones lag behind in areas where deficiencies in microphysical parameterizations and other small-scale structure representations can be depicted. New methods are currently under development.

The second challenge, closely related to the first, assesses forecast improvements and limits of predictability of current models. This is important when new observational networks are considered for improving forecasts, and costs of establishment and operation must be evaluated against a demonstrated level of improvement.

The final challenge involves practical utilization of information produced by deterministic storm-resolving models. A single forecast can be expected to have relatively little value because of high spatial and temporal intermittency of storm-scale events. Quantifying this value is highly problematic and is further complicated because the forecast contains no information regarding reliability. Using appropriate statistical analysis techniques, the ensemble can be made to yield probabilities over very specific time and space domains.

Related to the problem of characterizing space-time rainfall variability and predictability is the development of coupled hydrologic-atmospheric models that properly account for land-atmosphere interactions at a range of scales and, which can be used to assess effects of weather and climate variations on flooding and basin-scale water resources. This group is investigating the effects of subgrid scale variability of rainfall, topography, vegetation, and land use on energy and water partitioning via coupled modeling.

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Grain Sorting and Alternate Bars in Gravel-Bed Rivers

Two central problems in the field of river morphology are grain sorting and alternate bar patterns. This group is presently developing numerical models in these fields. A successful model of grain sorting and alternate bar pattern would provide the key to insight into a wide range of problems. Practical applications can also be found in these models. For example, the prediction and management of land use in watersheds and land use are two such applications.

The development of a unified model for one-dimensional sediment transport, downstream fining, and gravel-sand transitions is being focused on. For the most part, this topic represents a continuation of previous work. Three numerical models have already been created by this group that deal with different geomorphic problems in rivers. The group is now trying to unify these models into a comprehensive treatment applicable to natural streams as well as the laboratory.

Another focus is on the development of a two-dimensional model for sediment transport and alternate bars in rivers. Alternate bars are a common feature of gravel streams. While many researchers have studied the topic, little progress has been made in the area of numerical simulation due to the complications involved. Considering the importance of the phenomenon, both in regards to basic science and application, the group feels the time is appropriate to begin a full numerical model using recent theory and techniques they have developed. The theory in question was based on experimental results and field observations. The research revealed that a gravel front defining a transition to a sand-bed stream prograding into a subsiding basin must eventually be arrested. Numerical techniques used are derived from the simulation of aggradation and downstream fining as well as the computation of an arrested gravel front already reported on.

In the simulation, five to fifteen partial differential equations and dozens of linked algebraic equations must be solved simultaneously using iterative techniques. The expected results include the predicted patterns of grain sorting, topography, and flow pattern at both a local (bar) and global (reach) level. These results are being used to establish an elation between sediment transport, flow pattern, and stream morphology.

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Large Scale Computation of "Large Re-Small M" Industrial and Environmental Flows

There is no doubt that Navier-Stokes equations accurately represent real flows of Newtonian fluids such as air and water, but complete solutions of the Navier-Stokes equations for turbulent flows at large Reynolds number and complex geometry are still not attainable with state-of-the-art numerical techniques and computer facilities. This group is advancing the state-of-the-art for computational fluid dynamics and promoting its applications to industrial and environmental problems.

The first method of advancing the state-of-the-art is through the development of improved governing equations and boundary conditions. This group developed weakly compressible flow equations. These equations bridge the gap between aerodynamics and traditional hydrodynamics. Next, they developed the compressibility boundary layer theory. Combined with viscous boundary layer theory, this theory completes the bridging of ideal flow theory and real fluid flow theory. Inner flow is the compressible transient flow, and outer flow is the incompressible flow. Numerical solution of incompressible flow can be sped up by a factor of one hundred by using the weakly compressible flow approach. Last, they developed a single phase flow model for cavitating flows. By using a single equation of state for the liquid phase and the gas phase of water, various types of cavitating flows can be simulated without the need for the cavity closure condition, greatly simplifying the computation.

The second way this group is working to advance the state-of-the-art is through the development of improved modeling techniques and numerical schemes. First, these researchers developed a four-dimensional vector approach. By considering the three-dimensional unsteady flow as a general four-dimensional flow and by using the finite four-dimensional volume approach, it was possible to obtain a very accurate computational method for solving problems involving very rapid grid movement and deformation. Next, they worked on a simple large eddy simulation method suitable to finite volume approach. This approach shows that the effect of subgrid scale turbulence on large scale turbulence is very small except when the boundary layer separation point is very unstable. Next, a steepness limiting method and a smoothing method for simulation of free surface waves was developed. The final step was to develop a pressure smoothing method for the purpose of eliminating acoustic disturbances when the weakly compressible flow approach is used to simulate incompressible flows.

Currently, the group is developing a computer program to design the most efficient hydropower system with good cavitation characteristics. This dynamic model is being used to study flow separation and vortex dynamics with the help of numerical flow visualization. A local model is being used to study the characteristics of vortex cavitation at off-design condition and is finding possible means to reduce the effect of cavitation. Very fine grid system and large storage is being used to resolve the details of highly concentrated vortex flow. Other work in progress includes the validation of the computer code for the simulation of sheet cavitation and cloud cavitation on propeller blade like three-dimensional foils. Very extensive computations are being carried out, and the numerical results are being compared with available experimental data.

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Water Quality Simulations for Lakes and Streams Under Different Climate Scenarios

This research is developing and applying computational simulation methods that link hydrology, water quality, and biological habitats in lakes and streams to climate conditions. Cold regions, defined as regions where water bodies develop an ice cover, are a special focus of this research. Projected climate warming has a particularly strong impact on ecosystems and aquatic resources in cold regions.

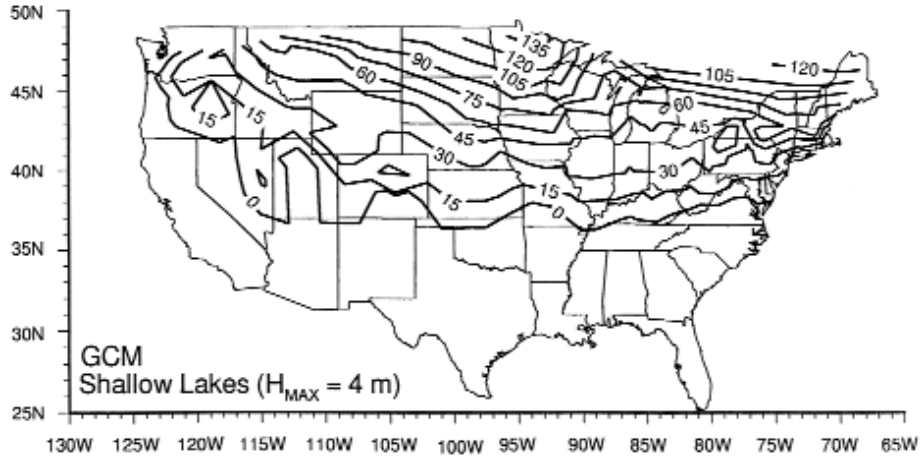
So far, deterministic, unsteady, one-dimensional, year-round lake water quality and fish habitat simulation models have been developed and applied in a continuous mode for many different types of lakes and long time periods. These models are complex by necessity but connect in very rational physical, chemical, and biological processes. These unique year-round simulation models can predict the water temperatures and dissolved oxygen concentrations in both the open water season and the ice cover periods and can determine ice-in and ice-out dates and ice or snow thickness.

The models are being applied to large sets of lakes in the contiguous United States. Lakes with different morphometries, primary productivities, and turbidities need to be simulated. Ice cover characteristics are quantified in lakes over the northern continental United States. Updated projected 2 x CO2 climate scenarios are available from GEMS (e.g., the Canadian Climate Center General Circulation Model). Sensitivities of simulation results to climate parameters still need to be established, and fish habitat parameters need to be simulated.

To support and validate individual model components, information has been collected on ice-covers and on snow and ice albedos.

The modeling efforts are currently being expanded to take the variability of water quality parameters across a lake surface into account. The exchange processes between near-shore and off-shore regions of lakes are being considered. The near-shore waters have more organic sediments, more rooted vegetation, and respond faster to atmospheric heat input. Consequently, on a daily or even seasonal timescale, littoral waters are different from pelagic ones. Two-dimensional mass and heat transport algorithms need to be developed and validated for this purpose.

The hydrodynamic model that simulates convective-diffusive-reactive exchange between shallow and deep waters of lakes has been developed and extensively tested. The comparison for the case of rectangular cavity flow driven by shear and buoyancy corroborates the fact that the model is highly accurate, stable, and efficient for a wide range of Reynolds and Grashof numbers as well as for different height to width cavity ratios. The model will be used as input for the prediction of diverse water-quality constituents (temperature, dissolved oxygen, nutrient content, and plant biomass) in lakes under different climate scenarios.



Simulated total days of ice cover per year on small, shallow lakes under the projected 2 x CO2 climate scenario.

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Unsupervised Document Set Exploration using Divisive Partitioning

Unsupervised clustering is a key component of machine learning, often used as a basis in data mining. This project is devoted to the development of a fast hierarchical divisive clustering algorithm. The underlying activity is the basic research needed to fully develop the divisive partitioning method and

the applied research needed to demonstrate its use on specific applications to make it easy for humans to use. Using the conceptual framework already developed, the goal in this project is to incorporate the finished parts into a variety of data mining applications while extending the information that can be extracted from the data. In addition, a user interface must be developed.

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Construction of Janko's Large Sporadic Group J4 Inside the Symmetric Group

Classification of finite simple groups is a major achievement in mathematics in this century. Unfortunately, its proof rests on many unpublished theoretical and computational results. Therefore, its revision is an essential project involving many research groups all over the world. This project is contributing to a comprehensive and well documented proof of the existence and uniqueness of the third largest sporadic simple group, J4, of order 86.775.571.046.077.562.880. The construction of J4 was announced in 1980, but the computational results were never documented.

In the project being undertaken by these researchers, the explicit permutations ï¿½(x) and ï¿½(y) require substantial disk space. This demanding, high-performance computation is constructing the largest permutation group ever dealt with in computer algebra. However, with these two permutations, researchers will be able to construct an embedding of J4 inside the 112-dimensional general linear group GL(112,2) over the field with two elements. Furthermore, they will be able to give a membership test for an arbitrary matrix M ï¿½ GL(112,2) to belong to J4. This small matrix representation allows every user a thorough and mathematically sound check of all the results obtained by means of the supercomputers on a small workstation or a personal computer using the computer algebra system MAGMA.

The German Research Council (DFG) has asked the Library of Gï¿½ttingen University to build up the German digital research library in Mathematics. It collects the digital mathematical journals, books, and also the mathematical databases of fundamental results. Because of the importance of the classification of the finite simple groups, the Gï¿½ttingen library has agreed to collect all the necessary digital data on the large sporadic simple groups like J4, the Baby Monster (BM), and the monster (M). Therefore, the two permutations ï¿½(x) and ï¿½(y) of J4 inside S173.067.389 and their correspondents inside GL(112,2) will be stored there. From the digital library at Gï¿½ttingen University, these data can be received everywhere over a high-speed network.

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Distributed Multimedia Computing

These researchers are currently working to providing viable solutions for issues involved in distributed multimedia computing. This necessitates both extensive simulations to validate theoretical results and substantial computing time on high-performance systems.

The first area of focus is on high-performance storage systems. To support multimedia networking/applications and high-performance computing, there is a growing need to devise new scalable architectures/protocols for server system/storage subsystems. Toward this end, the group is currently working on protocol and a performance study of serial storage architectures, fibre channel-

arbitrated loops, fibre channel-TORN proposals, and Aaron proposals. In addition, the researchers are also working with disk-based exclusive ORs, networked attached storage system/devices (Internet Protocol on storage devices), and scalable networking architectures for storage systems (fibre channel-arbitrated loop hub/switch design).

Another area of focus is multimedia networking and applications. A multimedia server capable of providing concurrent streams of video to multiple users is a critical component in a distributed multimedia computing system. The difficulty in providing multimedia with guaranteed quality of service is primarily due to the variation in access delays over the delivery path. First, the data has to be retrieved from storage, transmitted over a communication network to the end-user system, and finally displayed on the end-user system at a constant data rate. Each of the above components (i.e., storage, network, and end system) imposes a great challenge on the design and development of a multimedia server. This group is currently investigating different disk scheduling, disk placement, and video file striping schemes to study the performance of a mass storage system for a large-scale video-on-demand server.

The final area of focus in this project is integrated services over the Internet. The best-effort service paradigm of the present Internet is not considered adequate to support real-time multimedia applications. Hence, Internet Engineering Task Force (IETF) has extended this service model to include guaranteed and controlled-load services, where guaranteed service is intended for flows with tight real-time constraints and controlled-load service for adaptive real-time applications. To support such services, mechanisms for call admission control (CAC), traffic shaping, and packet scheduling are needed.

Previous studies have mostly focused on scheduling and admission control issues for each of these services individually. This group is investigating the interaction of these three service classes and its impact on the traffic and resource management. The goal of the study is to evaluate the efficiency of traffic shaping and admission control mechanisms in an Integrated Services network.

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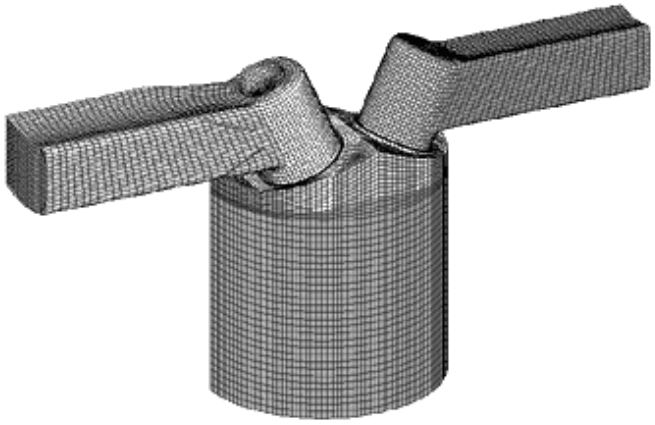
Scalable Parallel Algorithms and Libraries for Solving Large Sparse Linear Systems

These researchers are developing highly parallel formulations of key computational kernels used for solving linear systems arising in large-scale numerical simulations. Finite difference and finite element methods find extensive applications in scientific and engineering domain. They are used to solve problems in fluid flows, structural mechanics, wave propagation, electromagnetics, and heat transfer. Many linear optimization problems arising in logistics and control are solved using interior point methods requiring direct sparse linear system solvers.

The critical components of linear systems solvers are: scalable direct factorization, fast-high quality graph partitioners, and robust preconditioners amenable to parallelization. This group is developing a portable and parallel library for solving sparse symmetric positive definite (SPD) linear systems using direct methods. They are also developing new graph partitioning algorithms for problems arising in multi-phase computations as well as for use with robust parallel preconditioners. Using the elements of their direct solvers and graph partitioning algorithms, this group is developing parallel formulations of preconditioners for solving large sparse systems.

Existing methodologies for solving scientific multiphase computations on parallel computers suffer from either computational load imbalances between the various phases or incur a high communication overhead in transferring information between the various phases. This group is developing serial and parallel graph partitioning techniques to solve these problems and allow for the efficient parallel solution of multiphase computations. They are investigating two classes of parallel preconditioning techniques. The first class is based on the threshold incomplete factorizations. Even though threshold-based incomplete factorizations have been found effective, their parallel formulation on distributed memory computers are not well understood. This groupï¿½s preliminary parallel formulation makes use of their highly parallel graph partitioner and highly parallel algorithms for computing maximal independent sets to extract concurrency during the factorization process in addition to the application of the preconditioner. Their experiments have shown that these techniques are effective, but due to their small computational granularity, they are suitable only for architectures that have relatively low latency. They plan to develop new approaches of extracting concurrency that are suitable for

architectures and communication libraries with high latency. The second class of preconditioners is based on block diagonal preconditioners. In these preconditioners, a block diagonal matrix is constructed by ignoring any intra-domain interactions. A preconditioner of each block is constructed independently, and they are used to precondition the global linear system. The group is investigating computing a block diagonal preconditioner in parallel using a multi-objective graph partitioning technique able to simultaneously minimize the communication as well as the magnitude of the ignored interaction in the block diagonal matrix.



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

Two domains from an 8-way partitioning computed using the multi-constraint partitioning algorithm implemented in the Metis library.

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L1 Norm Algorithms and Minimization

In many important applications, a signal consists of a sum of exponential terms. The signal is measured at a discrete set of points in time with possible errors in the measurements. The signal identification (SI) problem recovers the correct exponents and amplitudes from the noisy data. An algorithm, Structured Nonlinear Total Least Norm (SNTLN), has been developed that can be used to solve the SI problem by minimizing the residual error in the L1 norm. In this work, the convergence of the SNTLN algorithm is shown, and computational results for two different types of signals are presentedï¿½one of which is the sum of complex exponentials with complex amplitudes. For comparison, the test problems were also solved by VARPRO, which is based on minimizing the L2 norm of the residual error. It is shown that the SNTLN algorithm is very robust in recovering correct values in spite of some large errors in the measured data and the initial estimates of the exponents. For the test problems solved, the errors in the exponents and amplitudes obtained by SNTLN were essentially independent of the largest errors in the measured data while the corresponding errors in the VARPRO solutions were proportional to the largest data errors.

It has been known for many years that a robust solution to an overdetermined system of linear equations Ax ï¿½ b is obtained by minimizing the L1 norm of the residual error. A correct solution, x, to the linear system can often be obtained in this way in spite of large errors (outliers) in some elements of the (m X n) matrix A and the data vector b. This is in contrast to a least squares solution where even one large error will typically cause a large error in x. In this work, the group gives necessary and sufficient conditions that the correct solution is obtained when there are some errors in A and b. A sufficient condition is also given for the more realistic situation where there are small random errors in every element of b and large errors in some elements of A and b. Finally, computational results are presented that give the probability, P, that a correct solution is obtained when there are large errors in k rows of [A | b], k <= m ï¿½ n. These results are presented in terms of an empirical relation that gives the value of m ï¿½ n needed in order to obtain the correct solution with probability P when there are k rows with errors.

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Parallel Iterative Solution of Large Sparse Matrix Problems

This group is currently developing algorithms, as well as software packages, for solving large sparse matrix problems that arise in certain applications. The first of these projects is the Parallel Sparse matrix Library (PSPARSLIB). This effort aims at producing software tools and methods for solving large sparse linear systems that arise in realistic applications. The second part of this project is an application in electronic structures calculations. The main problem here is to solve large sparse eigenvalue problems.

The first subproject is PSPARSLIB, an ongoing effort to develop a software package for solving general sparse linear systems on parallel computers. In PSPARSLIB, this group considers the most general framework of general (irregularly structured) sparse linear systems that are partitioned and mapped into a distributed memory multiprocessor system. The systems are solved with a preconditioned Krylov subspace technique. There are three major issues to be considered with care. First, the group is investigating preconditioning techniques developed specifically for distributed sparse matrices. These preconditioners must be as robust as their sequential counterparts. Second, reduction techniques for the impact of inner products in Krylov subspace accelerators are being looked at. These often cause parallel implementations to become inefficient. Finally, independent of consideration of parallelism, this group is pursuing a quest for robust iterative solvers with the goal of improving the current state-of-the-art.

On the preconditioning side, the methods to be developed are of three types: derived from a domain decomposition viewpoint but adapted to general sparse matrices, Schur complement related techniques, and methods derived from approximate inverses.

The goal of the second subproject is to develop computational methods that take full advantage of parallel processing in various forms to solve large scale electronic structures problems. This goal requires a rethinking and reevaluation of the traditional approaches devised for sequential environments. For example, the use of pseudospectral methods that employ Fast Fourier Transforms is to be avoided as these methods often present communication obstacles in parallel architectures. Rather, the focus of this work is on real space methods. The groupï¿½s emphasis is based on applying higher-order, finite difference techniques to the electronic structure problem. Finite difference techniques

coupled with ab initio pseudopotentials can provide a simple, yet accurate and efficient, approach to complex systems. The applications of interest center on electronic materials such as large clusters, liquids, and amorphous solids. Algorithm development within this context focuses on designing parallel preconditioners for the eigenvalue problem and the implementation of these techniques to various parallel platforms.

Currently, the group has a code running that uses Message Passing Interface (MPI). The code uses a master-slave approach in which most of the non-critical work is performed on the master node, and the diagonalization work is shared by all nodes. This model is being rethought and a fully distributed approach is being considered. Again, a critical issue is in finding good preconditioners.

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Ab Initio Simulations of Dense Plasma and Matter

This project centers on the development and use of highly efficient parallel algorithms and methods to treat fully quantum mechanical, three-dimensional systems of large numbers of strongly interacting atoms in dense plasmas and matter. To properly model the environments of importance, such as phase transitions, dynamically-altering constituents, and interpenetrating mixtures, requires very long-time simulations of thousands of particles. Density functional methods provide one of the most promising avenues for attaining such large-scale simulations. These methods use state-of-the-art numerical techniques to generate spatial wave functions from which a host of optical and electronic properties can be derived. The speed of these methods relies on two aspects: replacement of the nuclear coulomb potential with a non-singular representation or pseudopotential and utilization of fast iterative and sub-space eigen-solvers (planewave method), which do not require the construction of the hamiltonian and which scale as the square of the number of basis states, to obtain the electronic wave functions. Both facets can take particular advantage of the basic Origin-NUMA (Non Uniform Memory Access) architecture via OpenMP directives.

Quantum molecular dynamics simulations generate the needed information on structural, electronic, and dynamical characteristics of single components and convoluted mixtures of matter at high compressions and moderate temperatures. Such studies have a profound impact on many basic physics issues for these systems as attested to the many publications in numerous preeminent scientific journals. In addition, these systems play crucial roles in many weapons related cases from primaries as indicated in recent papers on the current controversy over the equation-of-state of hydrogen. The use of these computer resources allow a systematic and accurate exploration of such environments.
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Pen-Chung Yew, Principal Investigator

Parallel Computer Organization and Parallelizing Compilers

This researcher is designing large-scale, high-performance, distributed shared-memory multiprocessors (DSM) and their compilation technologies. The effort includes both development of an integrated parallelizing compiler for Fortran and C and high-performance memory system design for DSM. The development of an integrated parallelizing compiler allows both loop-level parallelization at the front end and instruction-level optimization at the back end. The high-performance memory system design is using compiler and architectural support to enhance data locality, reduce memory latency, and enforce cache coherence.

Another effort is leveraging multiprocessor technologies in the design of future generations of high-performance microprocessors. In particular, the design of single-chip concurrent multithreaded processors that support extensive speculative execution is being worked on.
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Mohamed-Slim Alouini, Principal Investigator

Performance Analysis of Noncoherent Reception over the Rayleigh and Nakagami-m Fading Channel

As the role of wireless communication becomes more important in society, the demands for these wireless communication systems increase. These researchers are working on these systems to achieve high-transmission rates with low bit-error-rates. In many circumstances, evaluating the error probability performance of optimum receivers is not possible by finding close forms of expression. Therefore, the simulation technique needs to be applied. In particular, Monte Carlo simulation techniques need to be applied to evaluate the exact BER or determine the accuracy of analytical approximations. In any case, these techniques and simulations require many computations and a large amount of computer time.

Research Group

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Model Selection Using Statistical Learning Theory

In recent years, there has been an explosive growth of methods for predictive learning in the fields of engineering, computer science, and statistics. The goal of predictive learning is to estimate (or learn) dependencies from (known) training data in order to accurately predict (unknown) future data originating from the same (unknown) distribution. Model selection is the task of choosing a model of optimal complexity for the given data. It is one of the key points to the success of predictive learning.

This research is focused on the fundamental issues as well as practical applications of model selection. This approach is based on Vapnikï¿½s statistical learning theory (SLT), a recent important theoretic

framework for learning with finite samples. Important contributions of this research include using optimal experimental design technique for accurate estimation of the VC-dimension that is the measure of model complexity in VC-theory and comparing VC generalization bounds for model selection for linear and penalized linear estimators with classic model selection methods. Others include a new structure for wavelet signal denoising based on model selection and the structural risk minimization principle as well as implementation and study of model selection methods for the new types of learning machines such as Support Vector Machine and Constrained Topological Mapping.

Research Group

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Stephen Chou, Principal Investigator

Optical Properties of Sub-Wavelength Dielectric Transmission Gratings

Sub-wavelength dielectric transmission gratings can serve as anti-reflection devices, wave plates, narrow band filters, and other optical elements. They are very attractive to future integrated optics because large arrays of different sub-wavelength optical elements can be made at different locations on a substrate using simple grating structures in a single fabrication step. Due to the fine period required, most of the previous investigations were theoretical, with the experimental studies few and limited. However, nanofabrication allows sub-wavelength gratings with periods as small as 50 nm to be fabricated with relative ease using electron beam lithography and reactive ion etching. For materials with small dielectric constants, effective medium theory and form birefringence theory accurately predict the optical properties of the materials. However, for higher dielectric constant materials, a different model is needed to simulate the grating properties. A simulation based on a rigorous modal expansion (RMS) theory can be used to predict the behavior of sub-wavelength period dielectric transmission gratings. The simulation operates by solving Maxwellï¿½s equations inside, in front of, and behind the gratings for an incident plane wave. From this, the eigenvalues and eigenmodes are obtained and coupled together to form the incident, reflected, and transmitted waves. Using the simulation, the reflectivity, transmittivity, and phase retardation can be obtained for incident light with polarizations both parallel and perpendicular to the grating fingers. By using this simulation, the properties of sub-wavelength gratings with different refractive indices, materials, thicknesses, and periods can be determined. This would allow researchers to both predict the behavior of gratings and to determine which fabrication parameters should be used to obtain gratings with specified properties.

Research Group

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Finite Element Modeling of Vertical Cavity Lasers and Integrated Optical Circuits

The Vertical Cavity Surface Emitting Laser (VCSEL) is one of the new laser structures developed in the past ten years. The great advantage of this structure is that standard microelectronics techniques may be used to fabricate the device, and expensive cleaving of the crystals and alignment of the facets normal to cleave planes are avoided. The disadvantage is that devices with diameters of the order of 10 mm and larger quickly become multimode, and the spectrum of emission has many lines. This group is conducting an experimental project to find means of keeping these single modes for all diameter sizes. To perform this project, the researchers are modeling these devices in considerable detail, and they are in the process of writing a vector wave solver in the cylindrical coordinates. They have written a code for current flow in p-i-n diodes, and this is being extended for the heterostructure diodes and will be extended to the cylindrical geometry. They have written a heat flow code, and this needs to be extended to the cylindrical geometry. They need to put these together for a self consistent VCSEL model. There are no such models available at this time.

In this project, they are experimenting with a new scalar edge element to solve vector electromagnetic wave propagation in dielectric guides. However, the tests on the scalar edge elements have been ambiguous, and it appears that they need to work with the vector edge elements in the cylindrical r-z geometry with rotational symmetry. A code has also been written for the current flow in heterostructures in the x-y coordinate system, and this is being debugged and converted to the cylindrical r-z system. This code solves the continuity equation with the Poisson equation using the Newtonï¿½s method of solving the nonlinear equations selfconsistently. A version of the temperature calculations of the VCSEL has already been written in Cartesian coordinates and needs to be converted to the cylindrical coordinate system. The group has also written a code for calculating the gain of quantum well structures with and without strain, and this is being used to calculate the gain of the wells with current drive. The rate equations need to be rewritten since earlier versions have convergence problems, and this is being addressed. The researchers hope to put all these programs together to run a self-consistent solver for the VCSEL. However, considerable time has to be spent getting all of the programs to work together.

The group is continuing work on an integrated optics project to go along with the VCSEL project. The current project includes integrated switch structures using semiconductor laser amplifiers as the switch elements, integrated semiconductor laser amplifiers Faraday rotation isolator, dielectric waveguide amplifiers, and dielectric waveguide amplified spontaneous emission sources. All these devices require waveguide mode solvers, with and without gain and loss, and in the cases of the Faraday rotation isolator, anisotropic media.

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Use of Heart Rate Variability to Improve Pacemaker Performance

In this study, wideband intraatrial and intraventricular electrograms are processed using heart rate variability (HRV) analysis. Parameters examined include Rï¿½R interval, Qï¿½T interval, depolarization slew rates, repolarization slew rates, depolarization amplitude values, and areas of depolarization curves in order to determine if useful information can be found in HRV analysis. The study is performed on asymptomatic pacemaker patients and congestive heart failure patients. Comparisons between measured parameters are listed, and suggestions for pacing algorithms are made.

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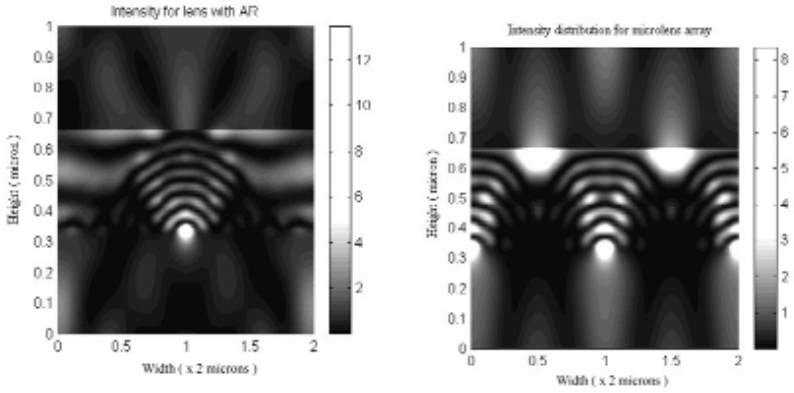
Analyses of a High-Power Solid-State Laser Cavity and Micro-Optical Elements

For many high-power laser applications, it is desirable to obtain the optical output in the form of a clean fundamental (TEM00) mode. The TEM00 mode has minimum divergence and minimum fluctuations of the emission due to elimination of competition between higher transverse modes. However, generation of heat in the active material of a high-power solid-state laser results in a transverse temperature gradient in the material that causes variation in the index of refraction as well as non-uniform stress birefringence. Thermally induced optical inhomogeneities in the active material affect laser output and are detrimental to efficient TEM00 operation. Unlike longitudinally-pumped solid-state lasers, phase distortions in side-pumped geometries are generally circularly asymmetric, complex, and cannot be easily corrected with conventional optics. This group has shown it to be experimentally possible to correct for an arbitrary complex beam distortion using diffractive optics. The element was designed as a phase conjugate of a measured phase error along the path of a mode and was fabricated using microelectronics fabrication techniques. However, the modal properties of the cavity are directly affected by thermal aberration in the gain medium and need to be investigated

numerically.

The cavity under investigation has a semi-confocal side-pumped geometry. The lasing material is a slab of YVO4 pumped from the side and cooled from the top and bottom. The resulting temperature distribution is clearly circularly asymmetric and results in a circularly asymmetric distorted beam. A two-dimensional computer model of the cavity has been designed. Including exact measured aberration profiles in the model has allowed these researchers to calculate mode profiles of the cavity and compare them with experimental measurement. They have also calculated modal gain discrimination of the cavity and have shown the cavity to be superior to a conventional design. With a computer model constructed by this group, further investigations are performed regarding the effect of the optimal location of the correction in the cavity, and general conclusions are drawn about the effect of simple aberration profiles (i.e., linear, quadratic, cubic, and higher order) on modal discrimination.

Properties of micro-optical elements are also being investigated. Many micro-optical elements have feature sizes too small for geometrical optics and scalar diffraction theory to be applied, making a rigorous solution of Maxwellï¿½s equations necessary. This group has written a MATLAB code based on the rigorous coupled wave (RCW) method to simulate two-dimensional periodic structures. The micro-optical structure is approximated by representing it as many dielectric slabs. More than one hundred slabs are required to simulate continuous micro-optical structures accurately. The Fast Fourier Transform (FFT) algorithm is applied to each slab to calculate the eigenmodes. For each slab, a one-dimensional FFT of 212 elements is used for convergence, and a 200 X 200 matrix is solved to find the eigenfunctions. A system matrix is then obtained by matching electromagnetic boundary conditions at the interfaces between every two adjacent slabs. The final system matrix has a size around 40,000 X 40,000. By solving this system matrix, the electro-magnetic field distribution inside and outside the elements can be obtained. For some calculations, iterations up to one hundred times are also necessary.



Electromagnetic field distribution inside a high index microlens array calculated by rigorous coupled-wave theory.

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Performance Enhancement of Heterogeneous Networks and Systems

Heterogeneous computing systems consist of dissimilar computers and, possibly, dissimilar interconnection networks. Research conducted on such systems has emphasized static task partitioning and dynamic task scheduling techniques to take advantage of the particular strengths of each of the heterogeneous systemsï¿½ compute nodes. In contrast, these researchers have investigated potential advantages obtained by utilizing multiple heterogeneous network types within a single system.

By establishing the relationship between message size and message transfer time for several types of networks, this group has found no single best choice for an interconnection network. Rather, the choice is dependent on the message size being transferred. For example, on the Silicon Graphics Challenge cluster, the group found that Ethernet transfers are faster than Fibre Channel when the message size is less than approximately 500 bytes. Beyond this point, Fibre Channel is the preferred method of transfer. They have found a similar relationship in the Shared University Research cluster for networks available on that system.

These preliminary results suggest that message-passing libraries, such as Parallel Virtual Machine and Message Passing Interface, can be augmented to effectively take advantage of more than one communications network by switching to the appropriate network based on the size of the message being transferred and, possibly, some additional parameters. Using multiple networks may also offer the added benefit of reducing the congestion in any of the individual networks.

To date, this group has developed techniques to automatically exploit the best features of each of the networks. For example, they have demonstrated on both the Silicon Graphics and IBM clusters that it is possible to reduce the total communication overhead of a parallel application program by switching between the two networks based on the size of each message sent. In addition, they demonstrated how to aggregate multiple heterogeneous networks into a single "virtual network" with an effective bandwidth that is approximately the sum of the bandwidths of the individual component networks. With its multiple types of interconnection networks, including Asynchronous Transfer Mode (ATM), Ethernet, and Fibre Channel, the Shared University Research cluster provides a rich environment to extend the evaluation of these techniques for reducing a parallel programï¿½s communication delays. The group is now developing a custom library for incorporating some of these techniques into programs from the NAS and PERFECT CLUB benchmark suites and the large micom ocean circulation model program.

This work has extended to simulating new types of computer architectures. In building new generations of microprocessors with ever increasing performance, computer designers always face two major challenges. The first is to tackle the scalability issue when increasing the number of instructions issued per machine cycle (IPC) while simultaneously shortening the clock cycle time. The second challenge is to bridge the worsening speed gap between the processor and its memory. These researchers have proposed the superthreaded processor architecture to address these challenges by exploiting more sources of parallelism in application programs through both instruction-level and thread-level speculation with compiler-assisted cross-thread runtime data dependence checking. One of the main goals of this project is to develop the new compiler technology needed to support the superthreaded architecture. Preliminary results show excellent potential for reducing application execution time with this architecture, but the results have also highlighted the need to more aggressively deal with the memory latency problem.

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Simulation of TURBO Decoder

TURBO decoder is well known for its very low bit error rate even at low signal-noise ratios. These researchers are working on the VLSI design of TURBO decoder as part of their project. Hardware architecture design is based on finite precision simulation. To test the very low bit-error rate (less than 10ï¿½6), these researchers need to simulate 108 information bits. Normally, this takes a Sun SPARC Ultra-10 machine one hundred hours to finish one sample. These researchers are currently working to simulate around forty different architectures.

Research Group

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Dennis L. Polla, Principal Investigator

Fundamental Study of Solid Acoustic Emission Microsensors

Fundamental properties of acoustic emission propagation in multilayered solid is under investigation by using microsensors. Since the microsensor is designed to detect the acoustic emission (AE) generated by fatigue crack formation and growth inside a solid material, acoustic transmission between a sample material and the AE microsensor is analyzed first. A linear and non-homogeneous matrix equation is employed to describe an acoustic wave traveling in the multi-layered thin film sensor. The matrix equation is solved by using a computer program. The reflection and transmission coefficients of longitudinal and shear waves between the sample material and AE micro-sensor are obtained from the theoretical modeling for a range of frequencies from 100 KHz to 1 MHzï¿½a typical frequency range of the AE induced by the fatigue cracks. The energy ratio of the reflection and transmission are

determined as well. To improve the acoustic transmission, a matching layer between the sample material and sensor is considered in the modeling. To monitor the AE, the sensor converts the acoustic pressure into an electrical signal. An equivalent circuit of the electromechanical transformation is studied qualitatively.

Research Group

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P. Paul Ruden, Associate Fellow

Properties of Semiconductor Devices and Materials

This ongoing research project is developing an understanding of novel semiconductor materials and devices. The two principal directions of activity currently are strain effects in III-V heterostructure devices and electronic and optoelectronic devices made from large band gap semiconductors.

The electronic properties of semiconductor devices are strongly influenced by built-in or externally applied stresses. Hence, there is considerable interest in developing a quantitative understanding of the strain distributions in realistic structures. This group has implemented finite element, mechanical analyses for a variety of devices. As part of this work, they have extended their investigation to strain effects in resonant tunneling devices and two-dimensional electron gas field effect transistors. The groupï¿½s current efforts focus on two-dimensional isoparametric finite-element analysis of crystal strains corresponding to a variety of conditions. Two-dimensional analysis is useful for studying elastic responses in certain simple model structures. Some realistic cases require three-dimensional analysis.

Additional work involves the study of III-Nitride compounds for possible use as new materials for high power electronic and short wavelength optoelectronic devices. The group has microscopically studied the dielectric screening properties of GaN and shallow impurity states in this material. Currently, they are running Monte Carlo electron transport simulations for AlN and GaN. They are also developing new device models suitable for these materials. Of initial interest are p-n homo- and heterojunction diodes as well as heterojunction transistors.

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Roger LeB. Hooke, Principal Investigator

Rheology of Basal Ice

The ability to predict the dynamic response of glaciers to a changing climate depends on accurate knowledge of the mechanical and physical properties of ice near the bed, which may be distinct from those of ice elsewhere. This research attempts to characterize the rheology of basal ice in a temperate glacier in Norway by means of field experiments and numerical modeling.

A wealth of experimental data obtained in the laboratory and on the surfaces of glaciers on the creep of ice indicate that the octahedral strain rate is proportional to the third power of the octahedral stress (e = Btn, n = 3). Therefore, models simulating glacier flow assume the ice behaves mechanically like a fluid with a generalized Newtonian constitutive equation with the viscosity function h given by the relation h = ao IIm/2, where II is the second invariant of the stretching tensor and ao and m are two material constants. The value of ao and m for temperate ice are not well constrained and depend in part on the water content and the ice fabric.

With the goal of determining ao and m for basal ice, an instrumented panel containing a conical obstacle was installed flush with the bedrock surface beneath Engabreen, an outlet glacier of the Svartisen ice cap in northern Norway, where tunnels in the rock beneath the glacier allow access to the glacier bed. Measurements of the sliding speed, by means of video cameras mounted behind transparent quartz-glass plates, and of the force the ice exerts on the obstacle, by means of a load cell mounted on the side of the panel, were obtained for two different obstacle shapes during two field seasons in April 1996 and November 1997. This data, together with a three-dimensional finite element model of ice flow, yield a consistent value of ao around 0.5 bar a1/3 (B = 0.9 bar a1/3). This is lower than other measurements by 25 to 100%. The determination of m proved more difficult, but present calculations indicate that m is between ï¿½2/3 and ï¿½1/3 (1.5 < n < 3).

Research Group

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Peter J. Hudleston, Associate Fellow

Rock Rheology and Deformation of Fold-and-Thrust Structures

Folds are good examples of ductile structures in which rock is deformed while remaining cohesive and continuous. Faults are structures that involve loss of continuity and brittle behavior. Despite these differences, both folds and faults are intimately related in natural deformed rocks. However, the relationship between the two is not well understood although there is little doubt that the two grow simultaneously. This project is working to understand how rheological and geometrical parameters influence shape of folds and strain distribution as one wall of a fault moves over the other non-planar fault surface.

Much of the previous work on this problem has taken folds to be the geometric consequence of movement of layered rocks over a non-planar fault. The most usual configuration is to consider a fault that is parallel to the layering in places called flats and where elsewhere cuts obliquely across layering in places called ramps. The folds that form as a geometric consequence of movement of the hangingwall over the footwall are termed fault-bend folds. The proposed work is focusing on the formation, geometry, and strain distribution on such folds.

This group is using a two-dimensional finite element method for slow (quasi-static) flow of an incompressible anisotropic nonlinear fluid. With appropriate choice of constitutive relationships, the code allows for the nodal positions to be updated after each time step to simulate fold-and-thrust deformation in non-linear rock materials and to compute cumulative strain in each element. The elements are linear convex quadrilaterals, and grids of at least 1,000 to 1,500 elements are used to represent a fold-and-thrust belt. Tens to a hundred or so iterations are required for convergence to a steady state velocity solution. This is done by solving a series of steady-state problems. The velocities at all nodes are calculated for the initial mesh and boundary conditions. An increment of time is chosen, and the distance that each node moves in this time is calculated. The nodes are then moved to their new positions and a new steady-state (quasi-static) solution is obtained. Cumulative strain and strain rates are calculated at each increment. The units of length, velocity, and time are non-dimensionalized by choosing the unit of length of the layer as the layer thickness and the unit of time as the time increment used to update nodal coordinates.

To facilitate a comparison, this group takes the footwall of the thrust to be nearly rigid and represents the hanging wall by a layered anisotropic viscous medium with different viscosities. The discontinuity that is the fault in nature is represented by a layer made up of very soft viscous elements in which large deformation is allowed. To avoid extreme element distortion in the fault zone, the group has updated the element grid as appropriate. Displacement on the fault due to forces or velocities applied to the boundaries of the model results in both a geometric change in the hanging wall and a dynamic instability due to the anisotropy. The geometry of the fault (e.g., dip angle of ramp), displacement on the fault, and degree of non-linearity of the hanging wall can then be varied to examine how these parameters affect the resulting fold geometry and strain variation in the hanging walls. The group is focusing on the effect of variations of dip angle of ramp and of competition of rock non-linearity on fault-related fold development in fold-and-fault belts. The results of the models are then compared with those in anisotropic materials and natural foldsï¿½in terms of the geometry of the folds, fold location with respect to the faults, and evolution of the structures with time.

Research Group

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Christian Teyssier, Principal Investigator

Finite Element Modeling of the Behavior of 2-phase Composite Materials

This project is studying the geodynamic role of mantle diapirs beneath mid-ocean ridges. Current debate among geologists, geophysicists, and oceanographers concerns the geometry of mantle flow beneath mid-ocean ridges and the mechanical and dynamical interactions of the rigid crust and mantle flow. The project focuses on the geologic evidence for three-dimensional mantle flow beneath ridges best exposed in one unique region on the globe, the Sumail Massif in northeastern Oman. Researchers working in Montpellier mapped and discovered this feature, interpreted to be the clipped head of a mantle diapir, exposed now as part of a slice of oceanic crust and mantle thrust up onto the Saudi Arabian continental margin. This group is currently studying these structures (chromite pods) deformed in the flow of mantle material, combining field work, experimental deformation, and finite element modeling of these structures at scales from less than a millimeter to tens of kilometers.

These rocks contain an example of a stronger material suspended in and deformed by a weaker material. The specific nature of this mechanical problem has roots in Metallurgy and Material Science, specifically in the study of the interactions of two phases with different strengths in composites. Finite element modeling allows this group greater freedom than either experiments or analytical methods alone, as they can vary scales, rates, and geometries of deformation to study the interaction of time dependent and time independent rheologies while keeping other variables constant. The estimation of rates of deformation (strain rates) from natural observations is a notoriously difficult task for phenomena that occur on geologic time scales. This use of finite element modeling to combine field and experimental observations provides a potentially powerful and little explored approach to this classic problem. From a series of numerical modeling experiments, these researchers are constructing estimates of strain rates and strain rate gradients in this structure and are building a three-dimensional image of diapiric flow. This larger image can be used both for studying stresses generated in the oceanic crust from the underlying mantle flow and for comparing to purely numerically generated three-dimensional fluid dynamic models of mantle diapirism.

A significant part of this project requires the improvement of the finite element toolï¿½s ability to simulate natural deformation of materials. Among the improvements this group is developing are an application of the remeshing technique to simulate large deformations, substitutions for creating discontinuities in an initially continuous mesh to simulate fracture, and ways to impose material anisotropies as boundary conditions. These techniques improve the physical representation of geologic processes. These are numerous examples of this mechanical problem in the earth and in the manufactured world. Engineers and Material Scientists are also interested in the strength of composite materials and the conditions of failure in one or both phases in the composite.

Research Group

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David A. Yuen, Fellow

Large-Scale Numerical Modeling of Geophysical Processes

This research is gaining a quantitative understanding of the Earthï¿½s interior from numerical modeling of complex physical-chemical and fluid-dynamical processes of time-dependent nature. The computational approach is two-pronged. On both powerful workstations and supercomputers of the PVP and MPP variety, these researchers initially study using two-dimensional models with complicated physics problems in order to map out the parameter space of interest. They then follow up with large, high-resolution, two- and three-dimensional calculations.

The first focus of this group is on three-dimensional convection of the Earthï¿½s mantle. The group has developed two numerical techniques. The first is based on spectral-transform methods and is extremely fast. The second is based on higher order, finite-difference methods and has spectral-like accuracy for integrating the time-dependent equations. Problems currently being studied with these techniques include thermal convection in the hard-turbulent regime in which there appear disconnected plume-structures, thermal convection with multiple phase transitions and depth-dependent viscosity, and thermal convection with temperature-dependent and pressure-dependent viscosity. Three-dimensional, thermal convection, high-resolution calculations using IBM SP computers involve up to eighty million unknowns at a given time-step.

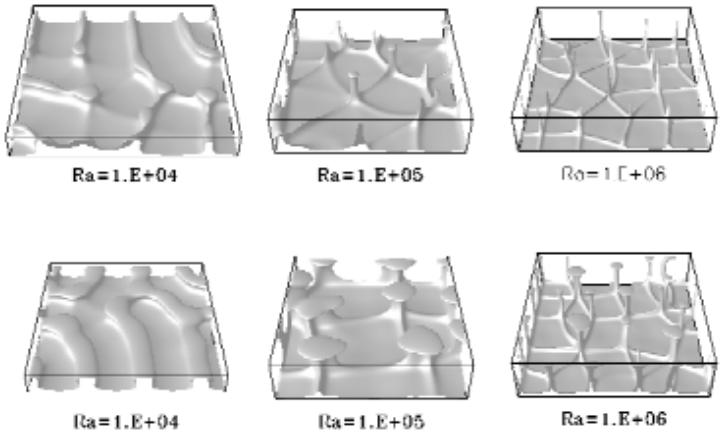
The second area of focus is on two-dimensional, time-dependent convection. The group is employing two-dimensional models for two reasonsï¿½to seek out and explore complicated chemical-physical processes with high enough resolution to capture the basic mechanisms and to conduct a reconnaissance search to explore a wider parameter space in new problems. Three types of numerical models are employed: bi-cubic spline method with the method of characteristics for the advection equation, finite-difference code with variable mesh and variable order capabilities, and a finite-element code based on a mixed second and third-order basis function.

A third area of focus is on the thermal history of the mantle in Mars, Earth, and Mercury. These problems are being studied by two-dimensional and truncated three-dimensional models. Megaplumes inside the martian mantle and their relation to the remnant magnetic field are the main target of this study. The numerical code for this research is based on finite-differences with variable order and variable-mesh capabilities. For both two- and three-dimensional models, core-mantle coupling is explicitly included by means of a time-dependent boundary condition at the core-mantle boundary that allows the core to be cooled. The physics of inner-core growth and radioactive heating are also included.

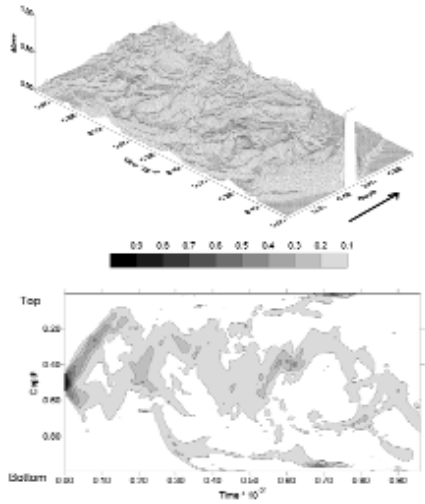
The next focus is on mixing dynamics using the method of lines and multifractal analysis and viscoelastic stress relaxation problems using an adaptive wavelet transform technique. Mixing in fluids is studied by following lines consisting of many passive tracers over one million. These tracers follow the trajectories of the velocities governed by thermally driven flow. Since a line is a boundary, this group can calculate many interesting statistical properties such as the length of the line, the fractal dimension, and the local Lyapunov exponent.

The last focus of this research is on the modeling of mesoscale hydrodynamical instabilities by large-

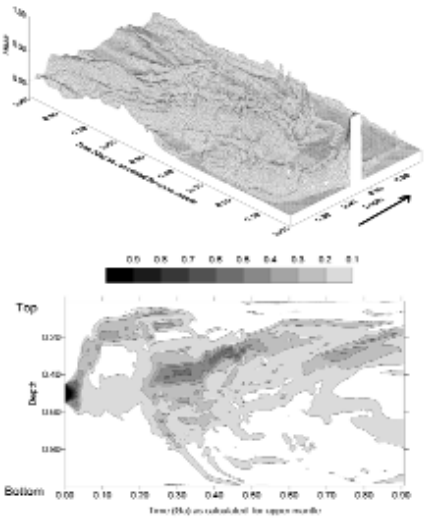
scale molecular dynamics and dissipative particle dynamics involving over one million discrete particles. Obtaining realistic results of hydrodynamic phenomena from simulations by particle methods requires computer codes to be adapted to enable simulations with the highest number of particles. This task requires modification of the existing codes and design of new algorithms. These researchers are currently in the process of adapting these codes.



Three-dimensional convection with radiative transfer k = 0.5 and with constant conductivity.



Mixing map of Newtonian convection. This describes the heterogeneity-time map and shows how the mass of the marker layer is migrating during evolution. The Newtonian pattern is destroyed within a short period of time.



Mixing map of non-Newtonian convection. Initial heterogeneity persists for a long time. Its spatial position remains relatively stable.

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Santiago Betelu, Principal Investigator

Asymtotic Solutions of Non-Linear Diffusion Equations

This work is concerned with convergent flows described by nonlinear diffusion equations. These equations may be used to model many important problems. For example, the study of gases flowing in a porous medium (as in an underground reservoir), viscous gravity currents on horizontal surfaces (as in a lava or mud spreading), and strong thermal blasts can all be studied using these methods. In the initial condition of this problem, there is a closed empty region surrounded by fluid. As time progresses, the fluid spreads into this region, and at some given time, the fluid fills the cavity.

The behavior of the asymtotic solution for the general two-dimensional flow is unknown. Only the circular symmetric case has been studied in detail. Moreover, recent experiments and computations suggest that the circular asymtotic solution does not always describe the general asymtotics of the problem.

In this work, this researcher is applying a novel numerical technique in order to solve this problemï¿½the numerical renormalization. In this method, the solution is renormalized each time the average size of the cavity reduces by a half. Essentially, the solution is rescaled, and the discretization is refined by a factor of two. With this technique, an accurate description of the flow very close to the collapse can be obtained, and the exponents that characterize the collapse dynamics can be computed.

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Bernardo Cockburn, Fellow

a posteriori L1-error Estimation for Parabolic Problems

This project is continuing a study of the quality of a posteriori error estimates for nonlinear parabolic equations in the L1-norm, the norm that should be used from the theoretical point of view when the parabolic problem is of a convection-dominated nature. Preliminary results indicate that the a posteriori error estimators are sharp. In this part of the project, the group combined the above mentioned error estimators with the so-called Local Discontinuous Galerkin method that has the main advantage of being a high-order accurate method with a high degree of parallelizability. The groupï¿½s main application is the compressible Navier-Stokes equations with high Reynolds numbers.

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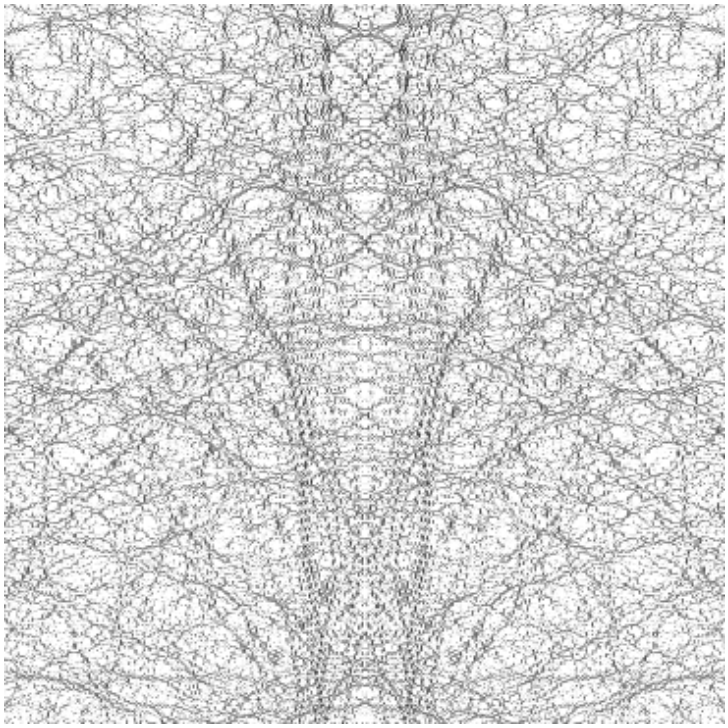
Computational Aspects of Analytic Number Theory

This group is using supercomputing resources to calculate automorphic eigenfunctions of the non-Euclidean Laplacian when the underlying Fuchsian group is one of Hecke triangle type. These eigenfunctions model quantum particles in Lobachevsky space. The codes being used are both microtaskable and parallelizable. The project is currently working to facilitate some benchmarking and possible revision of the basic algorithm. The end goal is to get all computational aspects operational and work toward implementation of calculation of the associated zeta functions (and similar functions).

The two figures show computer-generated images of quantum-chaotic eigenfunctions of very high energy in Lobachevsky space. The intricate patterns seen in these images are typical. Mathematicians do not yet understand why they exhibit the coherent shapes that they do.



The darkest grey regions show the places that the quantum "particle" visits most often, and the lighter grey regions show the places visited a little less often.

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Matthew G. Killough, Principal Investigator

Hysteresis and Metastability of Martensitic Microstructure

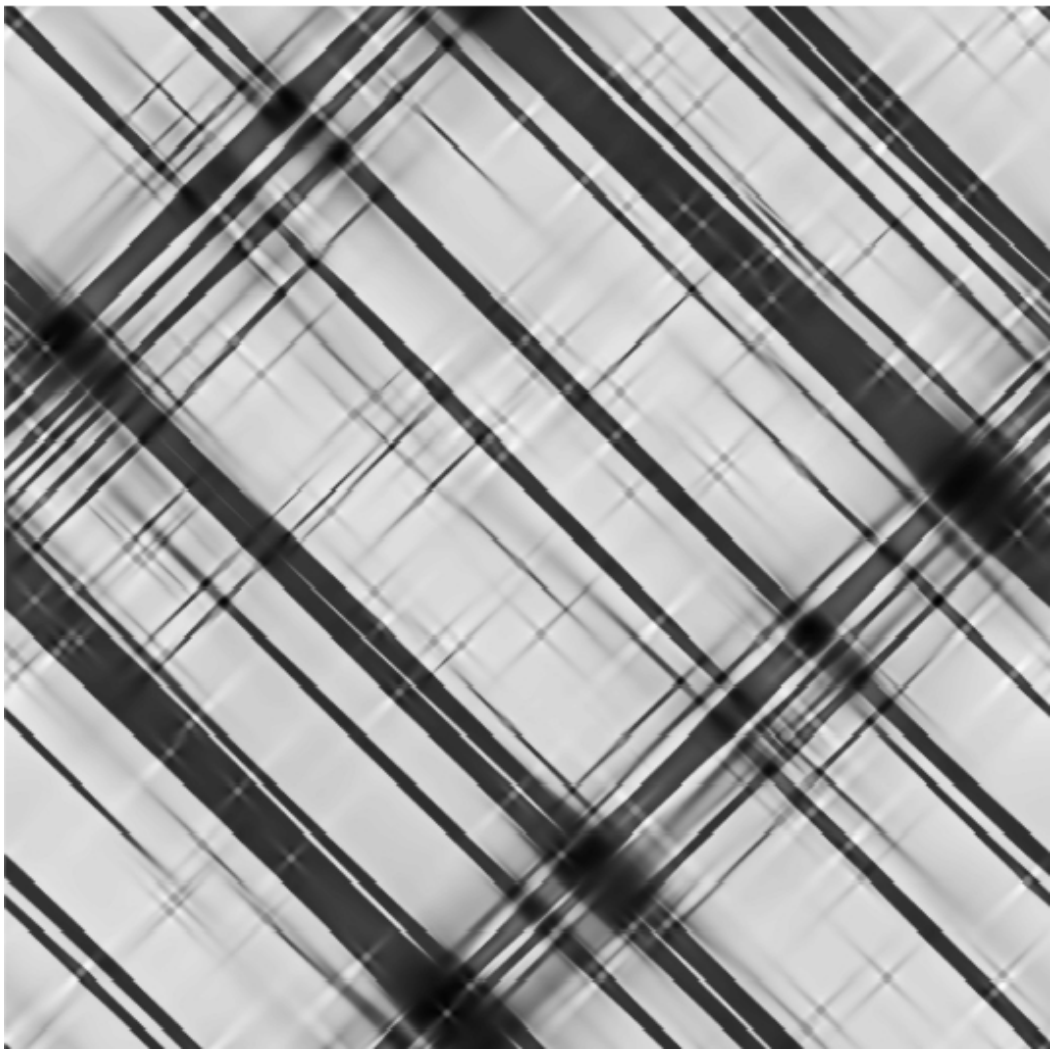
In a variety of solids, the molecular lattice undergoes a change of shape as the material is cooled past a specific transition temperature, Tc/i>. This so called martensitic phase transition typically involves a loss of symmetry in the lattice as the material cools from the high temperature (austinite) phase to the low temperature (martensite) one. Macroscopically, this loss of symmetry means that the martensite has a multiplicity of stress-free strains, called "variants" of martensite. Typically, the material organizes itself into a microstructure involving fine scale laminates of the different variants. In steels, for example, this microstructure gets locked into place and gives the steel its strength. This research focuses on another class of martensitic materials known as shape memory alloys (SMAs). In contrast to steels, SMAs have the ability to change their martensitic microstructure in response to applied forces giving them very unusual and highly nonlinear macroscopic elastic properties.

Although the elastic properties of SMAs are not very well understood, recent experiments at the University of Minnesota have shed some light on this subject. These experiments studied the response of a single crystal of CuAlNi to a program of dead loads. They discovered a hysteresis loop in the plot of the macroscopic deformation as a function of the applied load. The experiments clearly indicate that the kinetics of the microstructure controls the macroscopic response of the system. The conjecture was that an energetic barrier to the nucleation of new microstructural interfaces gives rise to metastable microstructures and causes the hysteresis, and that this nucleation barrier was the result of a competition between bulk elastic energy and surface energy at the interfaces.

In previous work, this researcher developed a model for the kinetics of the martensitic microstructure as well as an efficient numerical method for simulations using the model. The morphology of the microstructure that developed during the simulations matched the experimental observations very closely. However, the proposed nucleation barrier seemed not to be present in this model although the model took both elastic and surface energies into account. The simulations found no metastable microstructures, and although there was a hysteresis in the simulations, it was qualitatively different from the physical one.

Two distinct extensions of this model are being worked on. Each of these extensions has the potential to overcome the differences between the behavior of the model and the observations of the physical specimen. The first idea takes material defects in the form of non-transforming particles into account. The experimentalists report that compositional defects in the crystal give rise to small regions where the martensitic phase transformation never occurs. These defects should serve as nucleation sites for

new interfaces as well as barriers to pin existing interfaces in place. Thus, they would make it easier to form metastable microstructures and should have a large effect on the form of the hysteresis loop.



Strain during a simulation of stress-induced transformation from one martensite variant (white) to another (black).

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Topological Transitions and Singularities in Fluid Flows

The goal of this research is to refine and validate a physically-based method to capture pinch-off and reconnection in liquid/liquid interfacial flows. In fluid dynamics, changes in the topology of interfaces between partially miscible or nominally immiscible fluids are poorly understood. Such changes occur when continuous jets pinch off into droplets, when sheared interfaces atomize, or when droplets of one fluid reconnect with another. These transitions occur in many practical applications where reaction and mixing rates within the systems are controlled directly by the detailed dynamics of the transition processes.

Historically, the narrow zone separating immiscible fluids has been represented as a sharp interface. The classical Navier-Stokes equations can be solved on either side of the interface with the appropriate jump conditions prescribed across it. However, this sharp interface model breaks down and singularities form when interfaces pinch-off and reconnect. Furthermore, ad-hoc cut-and-connect conditions need to be prescribed in these models to evolve the flow through these events.

To overcome this difficulty, these researchers developed a diffuse interface model in which the sharp interface is replaced with a narrow, diffuse layer across which limited mixing occurs consistent with physical chemistry. This diffusion allows pinch-off and reconnections to occur smoothly and automatically and eliminates the need for cut-and-connect conditions. In this partial miscibility model (PMM), a mass concentration field, c, is introduced, and the model consists of a generalized diffusion equation (of Cahn-Hilliard type) for c coupled with the Navier-Stokes equations with extra stresses (due to ï¿½c) that mimic surface tension.

This group has solved several flow regimes in two dimensions using the PMM. Using a Boussinesq model, they have considered the flow of a jet aligned with gravity. They used parameters corresponding to an recently performed laboratory experiment. In this experiment, an axisymmetric jet of water/glycerin was pumped into a silicone oil ambient. The jet pinched off and the droplets oscillated downstream. The viscosity of water/glycerin is much lower than that of silicone oil. The group also numerically tested the reverse situation of silicone oil pumped into a water/glycerin ambient. For the experimental pumping rates, no pinch-off was seen.

The group also performed simulations of the PMM in a Hele-Shaw cell. In a Hele-Shaw cell, very viscous fluids flow between two closely spaced glass plates. The researchers found that the PMM also smoothly captures pinch-off and they are currently working to determine whether they can derive topological jump conditions from the PMM to supplement sharp interface models at the point of pinch-off and thus provide physically-based cut-and-connect conditions.

Currently, this group is moving toward more realistic simulations of topology transitions. They are focusing on axisymmetric and fully three-dimensional simulations. They are developing and testing new numerical methods to accurately and efficiently simulate these flows. Whenever possible, these results are being compared to actual experiments.

Further work is being done on computational problems in multicomponent and multiphase elastic materials. This is a continuation of studies that were done on microstructures formed in crystalline alloys. The group has been using both boundary integral methods and diffuse interface methods to simulate microstructural evolution in both isotropic and anisotropic media in two dimensions. The

group is currently exploring coarsening statistics for microstructures consisting of large numbers of precipitates.

Pinch off of liquid/liquid jet with c=0.5 contour surface.

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Computation of Active Martensitic Thin Films

This group is continuing to develop computational methods for nonlinear partial differential equations that model the dynamics of the austenitic-martensitic transformation in active thin films. The computation of active thin films is essential to the development of micromachines for wide-ranging applications from medicine to aerospace. The ultimate goal of this computational project is to develop the ability to simulate the behavior of shape memory materials, most of which undergo a martensitic transformation. The group is working to develop a computational model that can simulate the experiments currently being performed in the laboratory on a Cu-Al-Ni shape memory alloy.

Energy-minimizing sequences of deformations for martensitic crystals modeled by the Ericksen-James elastic energy density often exhibit a microstructureï¿½the simplest of which are layers in which the

deformation gradient is nearly constant and across which the deformation gradient oscillates between energy wellsï¿½to allow the effective energy of a deformation to be that of a macroscopic or relaxed energy. A more detailed model including a surface energy can be used to obtain a length scale for the oscillations and to select among competing energy-minimizing sequences, some of which may exhibit branching. During the past several years, this group has developed computational methods for the approximation of microstructure and a mathematical theory that has made rigorous analysis of the numerical approximation of microstructure possible.

The linearization of the dynamical model about some strains leads to an ill-posed problem since the energy density is not convex. However, the nonlinear model need not be ill-posed since the energy density is convex in the neighborhood of the energy wells where the deformation gradient is usually confined. A major goal of the computational program is to show how microstructure develops as a consequence of this ill-posedness.

These researchers are currently extending their model and numerical code to include thermal effects more accurately. They are using supercomputing resources to study the effect of the improved model on the propagation of the austenitic-martensitic interface. They are also working on simulating recent laboratory experiments that exhibit hysteretic phenomena.

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Three-Dimensional Pattern Formation and Shear Flow Visualization

The first part of this project deals with the visualization of patterns in three-dimensional fluid flows and

reaction-diffusion systems. These systems have been simulated. In order to visualize the results, movies of time-dependent patterns are made. These movies help gain an understanding of nonlinear dynamics and how geometry dictates evolution.

The other part of this project is concerned with visualization of three-dimensional velocity fields arising in complex geometries in particular channel flows with obstacles and sudden expansions. These researchers simulated these fluid flows and the project is now focusing on visualizing the results.

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Mathematical Model of Human Atrial Fibrillation

Atrial Fibrillation (AF) is a disease of the heart characterized by abnormally fast and irregular beating of the upper chambers, the atria, of the heart. If affects over 2 million Americans and, although not immediately fatal, it can lead to the formation of blood clots. It is the cause of about one-third of all strokes in people over the age of 65. Recently, an inherited basis was found when a gene was implicated in high incidence of AF within some families.

By combining biophysically detailed models of cellular electrophysiology with an anatomically detailed model of the human atria, this group is reconstructing electrical activity in normal and abnormal hearts. Currently, a system of 29 coupled, nonlinear, ordinary differential equations are being used to represent the "local kinetics" within each heart cell. At the moment, large two-dimensional sheets comprising a quarter of a million cells have been simulated in parallel on the supercomputers.

In addition to simulating the normal physiological function, this group is simulating chronic diseased states as well. Furthermore, the goal of the simulations is to explore options in patient therapies. One of these is called atrial ablation; this involves the controlled scarring of atrial tissue in order to disrupt the propagation of abnormally fast electrical waves. Here, the simulation of electrical activation can assist in the design of optimal ablation patterns. Electrical defibrillation is one alternative to ablation, but the large shocks needed to stop AF is associated with significant patient discomfort. Simulations may provide these researchers an optimal defibrillation strategy that could circumvent problems with currently available defibrillators. A third therapeutic approach is the use of pharmacological agents. The efficacy of drugs can be tested with simulations even before they are tried on patients. Recently, these researchers used numerical simulations to reinterpret the action of a whole class of heart drugs; the computational predictions were subsequently confirmed by experiments.

Further work in this group is being done on the collision of scroll wave filaments. This project is concerned with visualization of the topological changes that happen when scroll waves collide. The

researchers have simulated scroll waves in reaction-diffusion systems in two and three space dimensions. They are now working on bringing the results into a presentable format. A video is being produced that demonstrates the results and makes these results available in common movie format for the World Wide Web. In particular, the group is creating movies of a pair of scroll waves colliding due to periodic forcing, a scroll ring collapsing, a pair of scroll rings colliding to form a single scroll ring, and a tre fail knot transforming into a pair of scroll rings.

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Computational Approximation Dynamics

This group has been studying several global bifurcations for the Kuramoto-Sivashinsky equation (KSE) in detail. These bifurcations are triggered by the interactions between stable and unstable manifolds (one-dimensional and two-dimensional) of steady states and limit cycles. This approach is working to reduce the dimension of phase space by restricting flow to a three-dimensional approximate inertial manifold (AIM). Such a manifold can be described as providing a functional relation for the high (frequency) modes in terms of the low modes. There is strong numerical evidence to show that the local bifurcations for this reduced system are the same as that of the partial differential equations (PDE).

This group is seeking stronger evidence for the case of the global bifurcations they have observed. Their approach follows the theory of approximation dynamics. This theory requires the approximate inertial form to be a C1 perturbation of the PDE. If the C1 perturbation is small enough, certain hyperbolic structures are preserved under conditions quantifiable in terms of the linearized flow. However, to reduce the error for the AIM in some instances, one must increase the dimension of the manifold and lose the geometric understanding and low complexity of a three-dimensional phase space. In particular, by increasing the dimension of the phase space, one increases the dimension of the stable manifold making its computation unwieldy.

This group has implemented an algorithm developed to compute the inertial manifold to arbitrary C1-accuracy while keeping its dimension fixed. They have demonstrated convergence in a case where the exact manifold is known. With only a slight modification of the code, they successfully computed an inertial manifold with delay (IMd). This manifold enslaves the high modes at the present time in terms of the low modes at the present and the high modes at a small, fixed time delay in the past. Combining the IMd with multistep solvers for ordinary differential equations (ODEs), this group has demonstrated that they can compute a sensitive solution to the KSE as accurately in a three-dimensional phase space

as with using many modes in a Galerkin approximation. Then, the strategy is to find the initial condition for the reduced space using the original algorithm for the inertial manifold and evolve the solution using a scheme based on the IMd.

Now that the group can compute the solution on the inertial form to arbitrary C1-accuracy, they must do the same for the (un)stable manifolds of steady states and limit cycles within that reduced system. In particular, they need to obtain the angles the tangent planes make when two such manifolds intersect. The case where the manifolds are one-dimensional are not a problem because they are represented by a single orbit. In the case where the (un)stable manifold is two-dimensional, convergence of direct computational approaches can be complicated by a large gap in the associated eigenvalues that cause the flow lines to concentrate along the one direction. These researchers have developed a method to get around this by using ideas for evolving phase interfaces in the planes. The role of the interface is played by the boundary of the manifold in phase space. This group has implemented this approach on a test case (a simple ODE) where an exact form for the manifold is known.

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Thermal Management of High Heat Flux Electronics and Next Generation Packages

The first area of study in this work is heat sink optimization in natural convective heat transfer. Cylindrical pin-fin, longitudinal plate-fin, and longitudinal triangular-fin heat sinks are efficient in the thermal management of high heat flux chips. Past studies have analytically optimized vertical array geometries in natural convection. These researchers are using computational fluid dynamics methods to numerically model the hydrodynamic fluid flow behavior over different array geometries. The modeling is being carried out with ICEPACK and FIDAP programs. The group is currently validating past numerical results numerically and extending the investigation to horizontal arrays. The ICEPACK program is used to create representative pin-fin and triangular-fin models as well as the corresponding mesh. The preprocessing and solution of the meshed model are being solved using the FIDAP7.6 program.

The second phase of this work concentrates on immersion cooling. One of the methods proposed for cooling high flux electronic chips slated for use in the next generation of computers involves phase change of a dielectric coolant liquid on the chip surface. This efficient mechanism is often limited by the pool boiling critical heat flux, strongly affected by the chip thermal properties and thickness. Numerical modeling of the transient conduction process in the chip and the substrate is expected to yield a better understanding of the physics behind these effects. The Laboratory for the Thermal Management of Electronic Systems is pursuing ground-breaking numerical studies in the area of modeling vapor bubbles and their motion and hopes to apply subsequent findings to current experimental research. This is being done with spatial grids necessary to model very thin heaters as well as tiny vapor bubbles. Extremely small time transient solutions of two and three-dimensional models of the chip are obtained computationally. The group is continuing their investigations on the transient temperature distributions in the chip using a numerical finite element model. The time scales related to the critical heat flux (CHF) phenomenon require temperature solutions at very small time periods. In addition, the formation of dry patches on the chip during the boiling process induce large temperature gradients within the chip. As a result, very fine mesh sizes are necessary to accurately resolve these gradients. The transient temperature solutions are then used to understand the physics behind the effect of chip thermal properties on CHF and to validate some of the empirical parameters proposed in the literature to correlate the effect.

The last area of study is centered on thermal management of next generation packaging. The relentless improvements in semiconductor technology have continued to lower the cost of electronic systems and have created a nearly endless succession of new products. However, successful exploitation of future semiconductor technology requires significant improvements in packaging density and dramatic reductions in packaging costs. In response to these needs, the Packaging Research Center at the Georgia Institute of Technology is developing the Single Level Integrated Module (SLIM) packaging technology. As a part of research collaboration between the Laboratory for the Thermal Management of Electronics at the University of Minnesota and the Packaging Research Center (PRC) at Georgia Technical Institute, detailed thermal analyses of the SLIM package have been performed by using finite element codes.

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Stochastic Modeling and Simulation of Turbulent Reacting Flows

Computational fluid dynamics (CFD) is unique as a tool because it offers a detailed view of the flow phenomena that may otherwise be impossible. The field of combustion is one area that CFD has enormous potential. In performing calculations of turbulent reacting flows, there are three avenues that may be pursued: direct numerical simulations (DNS), large eddy simulations (LES), and Reynolds averaged Navier-Stokes simulations (RANS). In performing DNS, all relevant length and time scales are captured. This is the most robust methodology because no assumptions are made about the underlying physics or chemistry. It is a brute force method that yields the exact solution, but it is expensive. On the other end of the spectrum is RANS. These results are arrived at after a large number of mathematical assumptions that may not be correct. RANS calculations often fail to capture the time dependent features of the flow phenomena under consideration. This limits the problems that can be studied.

LES is considered somewhere between DNS and RANS because the small scale features of the flow are modeled while the large scale features are calculated explicitly. Relating small or unresolved scales to large resolved scales is the problem of turbulence closure. There has been relatively little effort to make use of LES for engineering applications compared to that in RANS calculations.

Schumann was one of the first to conduct LES of a reacting flow. However, the assumption to simply neglect the contribution of the small scale chemical fluctuations in this work is debatable. The importance of such fluctuations is well recognized in RANS computation of reacting flows in both chemical engineering and combustion problems.

One particularly useful approach in accounting for chemical fluctuations is based on the probability density function (PDF), the joint PDF, or the chemical species. This approach offers the advantage of having all statistical information pertaining to the chemical field embedded within the PDF, and any statistical quantity is readily at hand. The systematic approach for determining the PDF is determined by solving the transport equation governing its evolution.

The principal objective of this research is to make use of PDF methods to provide closures for LES of turbulent combustion. This is facilitated by introducing the filtered density function (FDF), and by providing an effective numerical means to simulate this FDF. Because of the added dimensionality of the compositional variables, solution of the FDF transport equation by conventional numerical methods is possible in only the simplest of cases. However, a Monte Carlo method may be used for this purpose. This scheme has proven very effective in RANS. Considering the capabilities and encouraging results in preliminary usage of this scheme, this methodology is being fully utilized for LES of turbulent reactive flows.

The most notable difference between the Monte Carlo solution of the FDF and the conventional procedures employed for LES is that the FDF accounts for effects of chemical reactions in an exact manner regardless of the speed of reaction and the character of the flame zone where it is unclear how to model the unresolved reaction rate in conventional LES. The advantage of FDF methodology over existing methodologies is the simple fact that the rate of chemical conversion appears exactly.

Stochastic particle number density in a turbulent round jet.

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Steven L. Girshick, Associate Fellow

Modeling Particle Nucleation and Plasma Synthesis of Materials

This research involves three projects. All three involve numerical modeling of industrially important systems in which thin films or particles are synthesized from the gas phase and experiments to which the models can be compared.

The first project concerns particle formation and transport in semiconductor processing systems. Low pressure thermal and plasma processes are used extensively in the microelectronics industry to deposit and etch thin films. Particle contaminants in such systems lead to defects and reduced product yield. Gas-phase nucleation is a major source of particle formation in these processes and may involve homogeneous as well as heterogeneous nucleation processes. This group is developing approaches for modeling particle formation and transport for these industrially relevant processes. The goal is to develop and integrate particle nucleation and growth models with transport models of the processing environment. Presently, these researchers are focussed on chemistries involving silane-hydrogen of silane-oxygen systems. These chemistries are used for chemical vapor deposition of amorphous and polycrystalline silicon films, for production of high purity bulk polycrystalline silicon, and for deposition of silicon oxide dielectrics. The group has developed detailed reaction mechanisms describing silicon clustering chemistry in these systems and has coupled these to models of the reacting flow and particle growth and transport.

The second project deals with chemical vapor deposition of diamond films in a thermal plasma reactor. Because of its unparalleled combination of superlative properties, there is extraordinary interest in diamond for a broad range of applications. In the past year, this groupï¿½s modeling efforts have been closely coupled to the experimental program. The SPIN/CHEMKIN II package was used to model the chemistry occurring in a gas chromatograph sample probe and the growth conditions in a newly designed reactor. The group has also developed two-dimensional models of the near surface region that account for the disturbance of the system due to sampling. Current modeling projects include development of a two-dimensional electrohydrodynamic model of the r.f. plasma torch used in the diamond chemical vapor deposition (CVD) process and in improving the treatment of surface chemistry in the one-dimensional modeling so that growth of different crystal orientations can be accounted for and predicted. The surface reaction model is partly based on results from ab initio and kinetic Monte Carlo calculations of diamond growth processes being carried out in the Chemistry Department. These efforts, together with experiments, attempt to define growth conditions that lead to

high-quality films and provide fundamental understanding of processes that govern film orientation, defect density, and growth rate.

The final project investigates synthesis of nanostructured materials in a thermal plasma expansion process. Nanophase materials show reduced sintering temperature, increased hardness, and interesting electronic and optical properties. This group has developed a process called hypersonic plasma particle deposition in which reactants introduced into a high-temperature plasma are supersonically expanded through a nozzle. This expansion drives nucleation of ultrafine particles, which are then collected on a substrate located downstream the nozzle by inertial impaction. Currently, the work is developing numerical models to simulate plasma flow and temperature distribution, particle nucleation and growth in the nozzle, and hypersonic deposition of these particles on the film substrate.

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

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Turbine Flow, Heat Transfer, and Numerical Simulation of Instantaneous Energy Separation

Gas turbine power and performance can be measurably improved by reducing leakage flow between the tips of rotating turbine blades and their encasing shrouds. Since the gap must be finite, flow rate through the gap is often controlled by altering the geometry of the blade tips. Heat transfer to the tip is also an important concern as the common problem of "tip burnout" severely limits blade life.

Using a modern low-Reynolds-number model of turbulence and qualifying mass transfer measurements in a mock-up rig, an experimental and numerical investigation is made into the simultaneous effects of inlet-side (pressure-side) corner radius on gap discharge coefficient and wall heat transfer rates. A sharper corner, by creating a large separation bubble at the entrance to the gap, should help to reduce tip leakage, but with an increased risk of tip burnout.

At least two cases of gap flow Reynolds numbers are being solved, one in the laminar flow regime and the other in the fully turbulent regime. The laminar case requires quite a refined grid in order to combat

numerical diffusion. The turbulent case requires the simultaneous solution of at least seven variablesï¿½two components of velocity, temperature, turbulent kinetic energy, turbulent dissipation, and two scales that deal with the turbulent transport of heat. The turbulent case needs to be run several times in order to optimize the model constants to fit experimental data.

With the numerical models matching the experimental results to reasonable accuracy, a systematic investigation into the effect of Prandtl number is then made. This requires at least one or two more computational runs for each case of Reynolds number.

Other work deals with numerical simulations of instantaneous energy separation. Fluids in motion separate spontaneously into regions with higher and lower total temperature. This separation, referred to as energy separation, can be observed in various types of flows such as shear flows, free, and impinging jets. Instantaneous flow and total temperature field are being numerically simulated to investigate the mechanisms of energy separation in shear and jet flows. The instantaneous pressure and temperature fluctuation within the flows provide the information for understanding of the mechanisms of energy separation.

However, the mechanisms of energy separation have not been understood clearly, especially the instantaneous mechanism of energy separation. In this work, instantaneous flow and total temperature field within shear and jet flows are numerically simulated. As the results, instantaneous velocity, pressure, and temperature fluctuations are obtained. These results provide useful information for understanding the mechanism of energy separation.

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Plasma Computation

The first project being investigated in this work is numerical simulation of the wire-arc spray process. Wire-arc spraying is becoming a popular process to apply metallic coatings to parts with a large number of applications in mechanical, automotive, biomedical, chemical, and electronics engineering. To improve the quality of the coatings, computer models may be used as design tools to simulate the complex interaction between magneto-fluid dynamic phenomena, turbulent transport, and molten droplet breakup. A three-dimensional code has been developed at the University of Minnesota to simulate the wire-arc spray process. This code calculates the compressible flow and temperature fields in the nozzle, torch, and jet of the system. A Lagrangian model is used to predict the trajectories, velocities, and temperatures of the molten droplets of the metallic wire as they travel from the electrode to the substrate. A sub-model is used to predict the breakup and resulting size distribution of the molten droplets due to the action of high-velocity and high-temperature plasma.

Another focus of this work is on computation of thermodynamic and transport properties of plasmas. The accurate calculation of thermodynamic properties such as enthalpy, specific heat and density, and transport properties such as viscosity, thermal, and electrical conductivities are required as inputs for a large number of computational and experimental calculations. In particular, for novel plasma processing applications such as reactive plasma spraying, accurate thermo-physical, and thermo-chemical data, mixtures of plasma gases is necessary. A computer code for the calculation of these properties has been developed and is currently being modified. For the calculation of chemical compositions and thermodynamic properties, an algorithm for the minimization of the Gibbs free energy is used while the calculation of transport properties is based on the Chapman-Enskog method based on solving the collision integrals.

The last project being looked at in this research is the modeling of r.f. plasma deposition process on a preform. The temperature and flow field in the r.f. plasma torch and the heating histories and trajectories of the particles injected into the plasma plume are modeled to simulate the actual deposition process. The behavior of a single particle and a large number of particles ranging from 50 mm to 300 mm are investigated. Radiation and carrier gas effects are also taken into account. SIMPLER algorithm is employed to solve the conservation equations of mass, momentum and energy, and the vector potential equations simultaneously. A low-Reynolds-number k-e model is used to model the turbulence in the plasma. Based on the calculated temperature and velocity distributions, particle heating histories and trajectories can be determined.

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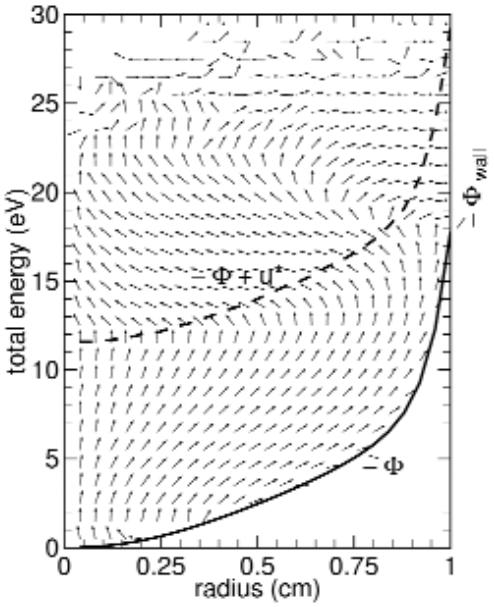
Highly Realistic Modeling of Electron Energy Distribution Functions in Gas Discharge Plasmas

A low-pressure plasma is a unique state of a gas in which chemically active species coexist with free charge carriers. Plasmas are produced by applying electric fields to gasses under low pressures of a few Pascal to several hundreds of Pascal. Plasma processes are widely used in microelectronics processing for etching of sub-micrometer structures and deposition of thin films. About forty percent of the total number of processing steps of modern microprocessors and random access memory relies on low-pressure plasma processes.

The increasing speed of new developments in semiconductor processing requires fast design of new plasma processing equipment. Currently, the design phase of a new plasma processing tool, which costs several million dollars, is limited to eighteen monthsï¿½its typical lifetime lasts about three years. Development of new plasma processing equipment proceeds empirically since no predictive computer aided design tools are currently available. Problems in computer modeling of plasmas are based on presence of multiple species and pronounced thermodynamic non-equilibrium of low-pressure plasmas. While heavy particles (ions and neutral gas atoms) have temperatures close to room temperature, the mean kinetic energy of free plasma electrons is of the order of a few electronvolt (i.e., their temperature is several ten thousand Kelvin). Precise prediction of plasma-chemical reaction rates requires accurate knowledge of the electron energy distribution function (EEDF).

This group is working on a project that focuses on the development of new, efficient methods for the calculation of the EEDF by approximate solution of the Boltzmann equation. To gauge the accuracy of these approximation methods, comparisons to rigorous methods based on first principles are necessary. The group is developing a fully self-consistent Monte Carlo code to calculate the EEDF in a low-pressure plasma system. They address the positive column of a direct current (DC) glow discharge as a benchmark system. Fully self-consistent treatment of the problem includes a five-dimensional Monte Carlo code for plasma electrons (three velocity dimensions and two dimensions in configuration space), a fluid code for plasma ions, and a solver for the Poisson equation. The code has been formulated as a parallel code using Message Passing Interface (MPI). First results of the code have revealed surprising details of the electron kinetics in positive column plasmas. The figure on the previous page shows the direction of the electron flux in a space spanned by the radius coordinate and the total electron energy. Surprisingly, the flux of electrons towards the wall is carried predominantly by low energetic electrons. At higher total energies, a flux reversal occurs, and the electron flux is actually directed towards the plasma center. The reason for this flux reversal can be seen in inelastic electron-atom collisions that act as an "absorption mechanism" for energetic electrons.



Electron flux in radius-total energy space in a positive column plasma in argon. ï¿½F represents the potential energy curve for electronsï¿½u* is the threshold energy for inelastic collisions.

Research Group

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Thomas H. Kuehn, Fellow
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Modeling and Numerical Simulation of Megasonic Cleaning, Filtration, and Ventilation

The first project being performed includes two parts. The first models the three-dimensional megasonic energy field in a specially designed, well instrumented megasonic cleaning tank. This type of tank is used to remove particles from the surfaces of wafers and electronic parts and to chemically process silicon wafers in a semiconductor manufacturing process. The second correlates cleaning efficiency (particle contaminant removal) with the local sound intensity distribution, the microstreaming field, and cavitation intensity distribution. The modeling method, calculated results, and final report provides Sandia National Laboratories and Semiconductor Manufacturing Technology (Austin, Texas) additional information for evaluating and improving megasonic cleaning systems.

The second project develops an asymmetrical, three-dimensional model for fibrous filters. This work is predicting the performance of real filter media used to remove aerosol particles smaller than 1mm in size. The flow in a filter media has been modeled by considering a three-dimensional module used to calculate fiber drag in the filters. Varying configurations of filter modules have been taken into consideration. The current objective is to extend the model to consider fibers of different shapes and

study the resultant effect on fiber drag. To consider the flow in real media, simulations for higher Reynolds numbers need to be extended (currently, simulations are in the Stokes regime, and this group is extending them to consider 0.1 < Re < 10). Also, the effect of polydispersity (fiber diameters of two or more sizes in the filter module) is taken into consideration to help simulate real media performance, and this is incorporated into the model. These simulations help resolve questions about the effect of three-dimensionality, fiber shape, and Reynolds numbers on the filter performance and increase the groupï¿½s knowledge on real filter media.

The third project continues work on the simulation of large enclosure flows. These researchers have obtained a good set of experimental data on such flows and have simulated such flows using various two-equation k-e turbulence models. The agreement between data and simulations is reasonably good for isothermal flows, but it is not good when significant density differences exist. The group thinks that large eddy simulation may be the best approach to predict the large-scale eddies observed in these flows.

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Francis A. Kulacki, Principal Investigator

Mass and Heat Transfer in Porous Media

These researchers have developed a numerical algorithm to investigate free and mixed convection in a horizontal porous layer media. Both natural and mixed convection are considered in a two-dimensional rectangular geometry. Time-dependent and steady solutions of the flow field and temperature are sought. The effects of Rayleigh number, the aspect ratio, and the length of the heated zone on the Nusselt number are being investigated.

Research Group

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Benjamin Y.H. Liu, Principal Investigator

Thermophoretic Aerosol Deposition in Turbulent Pipe Flow

Thermophoresis is the process where a temperature gradient causes a suspended particle to migrate in

the direction of decreasing temperature. Considerable work has been done to study this phenomena in laminar pipe flows. This study is concerned with how turbulent particle deposition and thermophoretic particle deposition interact within a turbulent pipe flow. Experimental studies have been performed that indicate the turbulent particle transport may enhance the thermophoretic particle deposition.

The first stage of this project is to generate the fluid flow field. Then, the particle deposition is modeled in the turbulent flow at no thermal gradients. Finally, the thermal gradients and thermophoretic deposition are included. The computational fluid dynamic program FLUENT has been used for this simulation work.

The flow field has already been generated. Turbulent particle deposition simulations and turbulent and thermophoretic particle deposition simulations have been run for different particle sizes and flow rates. The researchers have found that the turbulent deposition model overpredicts the deposition considerably. Current work includes focus on the turbulent deposition modeling by adjusting some of the dispersion parameters and deposition criteria by using the user-defined subroutines provided by FLUENT. When the turbulent deposition is considered reasonable, the cases including thermophoresis are rerun.

Research Group

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Susan C. Mantell, Principal Investigator

Finite Element Model of Wet Filament Winding

Filament winding offers great promise for manufacturing composite structures at reduced cost. During filament winding, continuous fibers that have been impregnated with a thermosetting or thermoplastic polymer matrix are wrapped around a rotating mandrel. The relationship between the crosshead speed V and the mandrel angular velocity w determines the fiber orientation or the winding angle j0. The tension of the reinforcing fibers F0 over the mandrel provides a positive radial pressure that serves to compact the previously wound laminate. These fibers are typically wound as tows (gathered strands of fiber) and may be wrapped in groups as adjacent bands. In general, the mandrel is cylindrical, spherical, or a cylinder with two hemispherical ends. More complex shapes can be wound depending on the winding head configuration and control (i.e., robotics head with multiple degrees of freedom).

A key manufacturing concern in filament winding is selecting materials and processing conditions to ensure final part quality. An analytic model of the filament winding process for wet winding of thermosetting matrix composites was developed. The model relates the processing conditions, part geometry, and material properties to the final part quality. Processing conditions include winding angles, winding speed, temperature, and tow tension. Material properties include resin kinetics and rheology, mandrel mechanical and thermal properties, and composite mechanical and thermal properties. Measures of final part quality include stress and strain in the cylinder during cure and after mandrel removal, final degree of cure, and final fiber volume fraction of each layer. The focus of the work has been on characterizing fiber volume fraction in wet wound cylinders. In wet winding, the

resin viscosity is stratified in the cylinder. Layers that have been wound first have the highest viscosity. Results indicate that the final position of the fibers is very dependent on the resin viscosity and the winding time. Model results also suggest that parameters that affect the resin viscosity and flow such as resin rheology, gel point, and fiber bed permeability must be well defined in order to obtain accurate model predictions.

This project is developing a finite element based model for wet filament winding. ABAQUS commercial finite element software provides the thermal and structural framework for the finite element modeling. Special user defined subroutines interface with ABAQUS to describe specific processes unique to filament windingï¿½the creation of layers, resin rheology and cure kinetics, and fiber motion including resin mixing. The result is a finite element based model that allows for viscoelastic materials, noncylindrical geometries, and multiple cure kinetics and viscosity relationships. The model incorporates several key features not included in the current (elasticity based) model including post cure, dome and joining geometries, and rubber insulating materials. The model structure is similar to the elasticity-based model. There is a thermochemical submodel, a fiber motion submodel, and a residual stress submodel. A post-cure submodel is then added.

Research Group

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Particle Nucleation and Growth in Semiconductor Vacuum Processes

In recent years, the focus of particle contamination in production of semiconductor devices has shifted from the clean room to processing equipment and toward smaller particles. For example, it is predicted that by the year 2001, particles down to 0.015 mmï¿½and perhaps as small as 0.005 mmï¿½will be critical to the yield of 1 Gbit DRAMS. Such ultrafine particles are typically produced by nucleation in the gas phase. The main objective of this research is to develop computational models to predict particle nucleation in Chemical Vapor Deposition processing tools.

This group is developing experimentally verifiable computational models to predict particle formation, growth, and transport in semiconductor applications. Although they have reliable models to predict the gas phase chemical information involved in these processes, their current understanding of nucleation in chemically reacting environments is inadequate. Specifically, the classical models do not account for complex chemical pathways leading to formation of stable clusters and subsequent growth involving heterogeneous chemical reactions on cluster surfaces.

An aerosol dynamics moment-type model coupled with a chemically reacting fluid flow model has recently been developed to predict particle formation in semiconductor processes. In this model, nucleation kinetics is modeled using a detailed kinetic chemical clustering mechanism. This mechanism provides the means to estimate the particle nucleation rate by solving a set of discrete chemical species mass conservation equations, which serve as the boundary condition to the coupled aerosol dynamics moment-type formulation. Relevant processes such as particle growth by heterogeneous chemical reactions and coagulation and particle transport by convection, diffusion, and thermophoresis are

included in the model.

Due to the complex chemistries involved in these systems (often > 30 reactions), only a simplified reactor geometry (between the wafer and the flow inlet) is solved. In order to understand the particle dynamics and transport in the complete reactor, the group has solved two-dimensional axisymetric fluid flow (with simplified chemistry) to predict particle transport in the whole reactor geometry.

Particle transport through the parallel-plate semiconductor process reactor for 0.04 mm (unity density) particles. The inlet flow rates for the four cases are: a) 100 sccm, b) 150 sccm, c) 200 sccm, and d) 300 sccm. The total pressure is 2.0 torr. The temperature of the wafer, showerhead inlet, and reactor wall are 750 ï¿½C, 200 ï¿½C, and 200 ï¿½C, respectively.

Research Group

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Computational Fluid Dynamics and Heat Transfer in Engineering Systems

This research is directed towards the development and application of numerical techniques for practical problems involving fluid flow, heat transfer, turbulence, and related processes. Computational techniques for flows in irregular geometries are being developed. These techniques are based on curvilinear nonorthogonal coordinates. The novelty in the technique is the absence of complication that normally occurs in the mathematical treatment of the equations. Cartesian velocity components are used to obtain the proper body forces and curvature terms in the momentum equations. Tests are being run to compare formulations with covariant and contravariant velocity components.

It is well known that the convergence rate of an iterative technique decreases as the grid becomes finer. By a suitable interplay of the original fine grid and a set of superimposed coarse grids, an efficient iterative technique can be treated. The development of such a technique for complex fluid flow is currently undertaken. Initial explorations show that speed-up factors of ten or twenty are easily achievable; even larger factors are possible for three-dimensional flows.

Thermal radiation is the most complex mechanism for heat transfer. Its exact distribution is governed by integro-differential equations. The radiation intensity depends not only on position but also on the angle. Numerical solution methods need to discretize the angular dimension as well as the space coordinates. A further complication is introduced by the absorption, emission, and scattering caused by the medium. Often, the radiation characteristics of the medium depend on the wavelength. When all physical details are included, the computation becomes very intensive. Methods are being developed for an accurate and economical computation of radiation heat transfer.

A class of interesting flow problems consists of solid particles or liquid droplets moving through a liquid or gas flow. The particles follow different trajectories depending on their size and density. In some situations, the presence of the particles has a significant effect on the underlying fluid flow. Novel techniques are being developed for the prediction of such flows. There are a number of possible industrial applications of this methodology.

Liquid flows often have a free surface of unknown geometry. In unsteady situations, the shape of the free surface may continuously change. A method is being developed for determining the shape of the free surface in a fixed computational mesh. The available methods in this area rely on explicit time-marching schemes and become computationally time-consuming. Often, implicit methods do not preserve the sharpness of the interface between the liquid and gas. The proposed method would retain efficiency of implicit schemes and still try to produce sharp interfaces.

The calculation of film cooling on turbine blades presents two challenges. First, the entire flow in the film-cooling hole (as affected by the upstream plenum) needs to be included in the calculation. Second, the film-cooling jets produce an anisotropic turbulence pattern, which is not predicted by standard turbulence model. Work is planned to introduce appropriate anisotropy in the turbulence model.

The flow and heat transfer in structured porous materials are calculated from first principles by solving the governing differential equations for the flow and temperature. From these computations, the effective properties of the porous material are obtained as a function of different parameters characterizing the material.

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Pleated Panel Filter Optimization Under Particle Loading and Nanometer Particle Filtration

Panel filters are used in industrial and residential applications. To allow more air flow through filters, the filter media in panels are pleated to increase the filtration surface and reduce the face velocity through media. However, the pleat spacing will be reduced when more media are pleated, and this results in pressure drop increase due to viscous force. Therefore, a well-designed panel filter is one that gives low-pressure drop and high-filtration efficiency. A low-pressure drop panel filter with high-

filtration efficiency results in significant energy saving for operating blowers/pumps used for fluid recirculation through filters.

In reality, most commercial filters are used under dusty environments. When dust is loaded on filters, pressure drop is increased due to the change of filter properties under the depth filtration condition or due to the narrowing of pleat channel under the dust cake filtration condition. These researchers are optimizing the pressure drop across panel filters under particle loading conditions using computer simulations.

In this study, the finite element method with the 27-node Lagrange element (velocity-pressure element in three dimensions) is used to solve Navier-Stokes equations in the region outside of the filter, and the Darcy-Forchheimer-Brinkman (DFB) model is applied to the filter media. Because of the nonlinear effect of filter media and the iteration process for fluid flow, the overall iteration process for nonlinear behavior of filter media is needed. In order to reduce computational time, the algorithms suitable for multiple processors will be implemented to solve the linear algebraic equations constructed from the finite element formulation.

To investigate filter pressure drops under the dust loading conditions, particle trajectory equations, including the diffusion mechanism, is used to predict particle concentration distribution along the filter medium surface in the upstream. Monte Carlo simulations are needed for this prediction due to the involvement of the diffusion process. Furthermore, particle deposition inside filter media is predicted by a model. It requires a calculation of loaded filter media properties for each composed finite element based on the local air velocity.

Other work is dealing with nanometer particle filtration. In predicting nanometer particle penetration through filter media, two defects have been detected in the published modelï¿½lack of considering particle multiple bouncing on the filter surface and examinating on the assumption of the particle impact velocity distribution. Monte Carlo simulations are being used to resolve these problems.

Following the filtration theory of single fiber, filter media can be represented by cell assembly. Many cell models assumed circular outer boundaries for ease in implementing boundary conditions. However, it raised the question on how to assemble this type of cell into an entire filter media. This group has developed a natural cell model that removes this dilemma and the method can be applied to cases of non-circular fiber cross section.

Individual particle with initial velocity assumed to be the same as the local flow velocity is being released into a cell from positions along the cell outer boundary. By tracing individual particles down, these researchers can simulate the filtration process if the collision model is included. Once the particle density along a fiber boundary is obtained, the single fiber efficiency can be easily calculated by integrating the density along the velocity phase and the fiber boundary. Then, filter efficiency can be evaluated using single fiber filtration theory.

Research Group

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Large Eddy Simulation of Turbulent Flow and Heat Transfer in Propulsion Systems

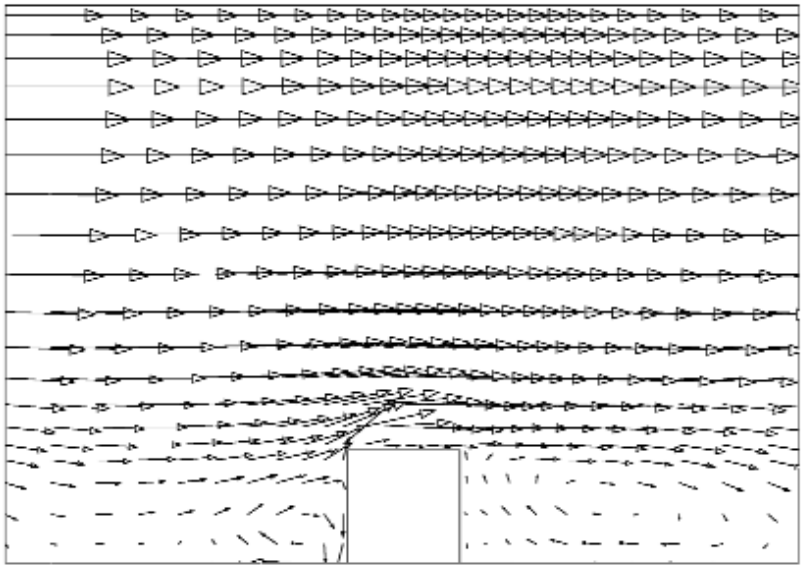
Recent work has developed algorithms and methodology for direct numerical simulations (DNS) and large eddy simulations (LES) of turbulent flows with heat transfer using a compressible formulation of the Navier-Stokes equations. This approach to DNS and LES is thought to be somewhat novel in three respects. First, there have only been a few studies reported to date in which a fully coupled, compressible formulation has been for either DNS or LES. Second, an all-speed strategy is being followed in the numerical simulations that permit the same general methodology to be applied to fully incompressible flows, compressible flows at very low Mach numbers where effects of property variations need to be accounted for, and at transonic and supersonic speeds. Basically, this flexibility is achieved by employing a coupled, compressible formulation with low Mach number preconditioning. Third, effects of heat transfer are being considered. Although some heat transfer results have appeared, available results are very limited, especially for separated flows, and usually do not take effects of variations in fluid properties into account.

Flows of interest include film and internal passage cooling flows in turbines and transition of the type occurring in low-pressure turbines operating at low Reynolds numbers. Over the past several decades, turbine inlet temperatures have increased significantly as higher efficiencies have been achieved. Achievement of further improvements in engine efficiency is largely dependent upon further increases in turbine inlet temperatures that place even greater demands on blade cooling procedures.

In numerical simulations, it is possible to impose temperature differences, heat flux levels, and even rotation effects difficult to establish in experimental programs. Thus, LES offers a way to gain fundamental information about turbine cooling flows to augment what can be learned from experiments. Such information can be used to refine turbulence models for use with the Reynolds-averaged equations.

Design criteria for gas turbine engines tend to result in maximum efficiency under takeoff conditions. However, at cruise conditions, Reynolds numbers are lower, and effects such as transition and bubble separation often result in a deterioration of turbine performance. Physics of such flows and effects of passing wakes is neither well understood nor accurately represented by current models. Here again, DNS and LES can reveal aspects of the fundamental physics of such flows, providing details that are not easily measured experimentally. Such information can guide refinement of turbulence models for use with Reynolds-averaged equations.

Significant progress has already been made. A strategy has been developed for LES using zonal embedded grids that reduce the number of computational cells required to achieve a given accuracy. This results in a reduction in computational effort and is very important because required computational effort is the pacing item that limits the use of LES for solving applied problems. In addition, two very promising schemes have been developed for avoiding solution decoupling that sometimes occurs at high Reynolds numbers. For LES, the use of traditional smoothing causes a serious deterioration of solution accuracy. The new methods effectively filter troublesome grid scale oscillations from results without otherwise damping the solution.



Velocity vectors showing flow pattern obtained from the large eddy simulation of a turbulent flow through a channel with a rib-roughened wall.

Research Group

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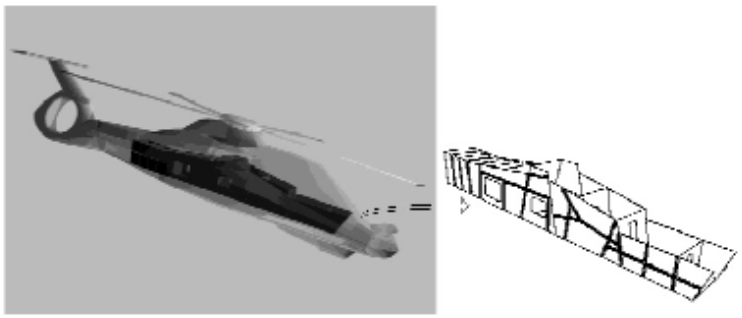
Kumar K. Tamma, Fellow

Integrated Process Modeling and Interdisciplinary Computational Mechanics

This work is developing integrated modeling and testing simulations in a concurrent engineering environment for process modeling simulations during composites manufacturing by net-shape processes and subsequent testing to withstand design and service loads. The process modeling of composite manufacturing processes involve flow, thermal, and reaction kinetics during the manufacturing process. The successful manufacture depends on the interaction of the complex phenomena during the process. Numerical methods, the finite element method in particular, form the basis of the process simulations as well as the subsequent integrity analysis to withstand the design and service loads. For a detailed analysis of complex engineering structures and designs involving accurate modeling of geometrical, physical, and material variations, physical models composed of several thousands of degrees of freedom are being used and are becoming common. This work is targeted toward implementation and development of physics-based simulations on the symmetric multi-processing computing system of the Origin 2000. While the physical and mathematical models and the numerical methodologies employed in the physics-based simulations may remain the same, the

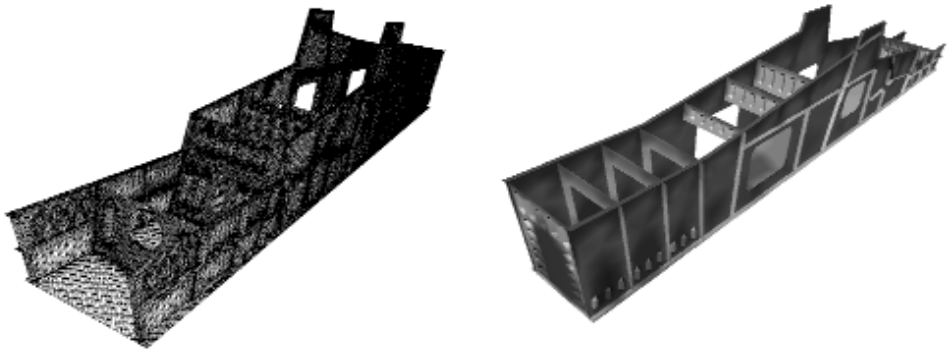
implementation and development of the physics-based simulation software on different high-performance computing platforms differ widely. This work is providing optimal solution algorithms, data structures, communication and computation strategies for efficient implementation of physical simulations on these symmetric multi-processing computing architectures.

The second part of this work constitutes an effort by these researchers toward the development of unified computational methodologies, solution algorithms, and finite element modeling and analysis strategies for interdisciplinary flow-thermal-structural problems. The philosophy and rationale advocated in the present study is based on employing a common numerical methodology for each of the individual disciplines in conjunction with common computational algorithms for applicability to supercomputing systems in solving large scale engineering problems. Various research activities include the development of new time integration algorithms for transient problems, development of effective finite element based methodologies that can be used in multidisciplinary problems, new physically correct contact models for penetration and impact problems, application of finite element methods in the manufacturing simulations, and providing a paradigm for Virtual Manufacturing. The application areas include a wide range of engineering applications involving metal forming, casting, thermal degradation, and composite material processing. The overall efforts focus attention on providing new and effective approaches for not only improving the existing capabilities for applicability to supercomputing environments, but also toward providing an accurate understanding of the physics and mechanics relevant to multi-disciplinary engineering problems.



Commanche keel beam

Commanche keel beam used for advanced composites modeling and simulation.



Finite element mesh of keel beam

Fill contours

Advanced composites process modeling and simulation of a Commanche keel beam. The left figure shows the finite element modeling mesh of the beam, and the right figure shows the same beam with fill contours.

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Computation of Chemistry and Physics of Nanoparticle Growth Processes

These studies are using molecular based computation to understand the growth of nanoparticles from the vapor. The application is toward the formation of new materials and the control of the emission of toxic heavy metal particles from combustors. These studies employ three theoretical approaches.

The first approach uses classical molecular dynamics simulations to understand particle-particle interactions and properties. Specifically, these studies are aimed at determining particle-particle reactivity and physical/chemical properties of small particles (surface tension, internal pressure, etc.).

The second approach uses ab initio molecular orbital methods to construct thermochemical databases and reaction rate data for the construction and testing of reaction mechanisms for reacting flows. The primary tool employed here is the GAUSSIAN suite of programs.

The final approach uses the results from the molecular dynamics simulations and ab initio computations to feed reacting flow simulation programs aimed at simulating particle forming flows. These simulations employ the CHEMKIN suite of programs and are used in simulation of combustion and chemical vapor deposition processes.

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Department of Astronomy

Thomas W. Jones
Evan D. Skillman
Paul Woodward

Thomas W. Jones, Fellow

Numerical Studies of Particles and Fluids in Astrophysics

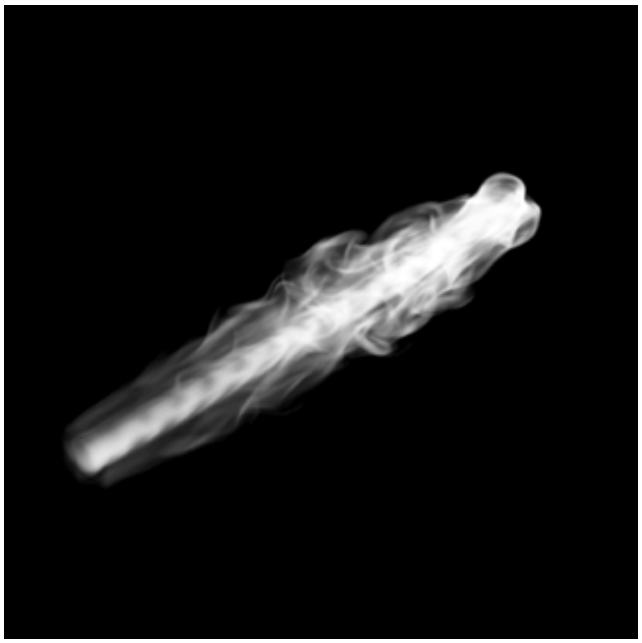
This research continues a very successful pioneering program in computational astrophysics. The program is centered on improving the fundamental understanding of the behaviors of high-energy charged particles (also known as Cosmic-Rays) and magnetic fields in cosmic plasmas and the application of this knowledge to the understanding of some recognized key astrophysical problems; namely, the origins of the cosmic-rays, the nature of giant radio galaxies, the nature of supernova remnants, and the nature of the interstellar medium in our galaxy. The specific work under current progress is carrying out two significant simulations based on state-of-the-art codes for compressible magnetohydrodynamics (MHD) and novel schemes for following the acceleration and propagation of cosmic-rays.

The first part of the work involves carrying out the first three-dimensional MHD simulations of particle transport and radiation from radio galaxies. These simulations include the acceleration and transport of the relativistic electrons producing the observed emission. This is an extension of the two-dimensional MHD simulations already completed. This is an important step that allows, for the first time, modeling a direct connection between the flow dynamics of the jets driving the phenomenon and observed properties of the objects. These are the first calculations that allow a real test of the basic hypotheses used in the field. The extension to three dimensions is important because it allows the researchers to drop the limiting assumption of axis-symmetry in the jet flow and allows for the proper full development of three-dimensional turbulence in the magnetized back-flow of the jet material. This is the primary region of radio emission, and the emission is highly sensitive to the strength and structure of the magnetic fields. The group is currently carrying out a high resolution simulation on a 3842 X 768 grid. The calculations need to be continued for at least twenty dynamical times. Because of the very complex dynamics in these flows, and the importance of capturing that for proper determination of the magnetic field evolution, it is important to include simulations of the highest spatial resolution possible. The simulations include momentum dependence to the relativistic electrons so they are effectively four-dimensional.

The other part of the work centers on three-dimensional MHD simulations of supersonic cosmic plasma clouds. This group has carried out the first two-dimensional MHD simulations of the evolution of supersonic gas clouds in the interstellar medium, and more recently completed a detailed study of collisions between such clouds. Statistically, such collisions are supposed to happen about once in a million years. This groupï¿½s studies have shown that if magnetic fields are absent, these clouds are largely disrupted individually. However, they found that even a modest magnetic field can be a very important stabilizing influence. In fact, in two-dimensional simulations, the field may effectively shield the clouds from almost any dynamical destruction. If this is really valid, it has profound implications for the structure of the interstellar medium where there is a small but significant magnetic field. This work is being extended to three-dimensional flows using the codes developed by this group. Only in

this way can they establish the importance of the two-dimensional symmetry assumed in earlier computations. The group has speculated that if clouds have a roughly spherical shape, magnetic fields may be largely shed, but a sausage shaped cloud may be able to hold onto the local field to build it into a shield. Currently, the group is carrying out high resolution three-dimensional MHD simulations of interstellar clouds.

The third area of recent effort has been development of new computational tools for the simulation of particle transport and acceleration near shocks. Accurate treatment with realistic parameters is technically very challenging, since it requires spatial resolutions ranging over several orders of magnitude from the physical thickness of the shocks. The group is introducing, for the first time, adaptive mesh refinement techniques and sub-zone shock tracking into this problem. This will also enable a more physically complete treatment of the injection of nonthermal particles from the thermal plasma population at shocks. Early results are very promising.



Synthetic radio emission image of a simulated cosmic hypersonic plasma jet. The three-dimensional magnetohydrodynamics simulation was the first of its kind to include explicit transport of high-energy electrons that produce the observed radio emission in cosmic "radio jets."

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Evan D. Skillman, Associate Fellow

Steps to the Primordial Helium Abundance

The value of the primordial helium abundance, the fraction of baryonic matter converted to helium in nucleosynthesis shortly after the Big Bang, is an extremely important constraint on current cosmological models. The amount of helium created constrains the total mass density and rate of expansion of the Universe. An upper limit on this value comes from measuring the helium abundance in emission line nebulae of metal poor dwarf galaxies. Such galaxies, with a gas reservoir relatively unpolluted with the nucleosynthetic products of stars, yield the lowest known helium abundances.

Since the variation of helium abundance with cosmological parameters is small, it is important to constrain this value to within one percent or so. Since the brighter helium emission lines in these galaxies can now be measured with an accuracy of this level, it remains to be determined whether the steps required to convert these emission lines to abundances are also secure to within one percent and to limit the systematic uncertainties. To this end, this group has carried out the most accurate calculation to date of the helium emission spectrum, including several improvements in the atomic data over previous calculations. In addition, this group has attached an uncertainty to the predicted emissivities for the first time based on assessment of the quality of the input atomic data.

The group then compared the results of their calculations to the observed helium emission spectra in three nebulae. While their calculations yielded better agreement with the data than previous work, there still remained several discrepant lines. Some of these discrepancies are almost certainly due to radiative transfer effects; absorption of nebular photons by the helium atoms in a metastable state alters the recombination cascade and the resulting intensities.

This group has developed fitting functions to the atomic data that allow them to calculate the emissivity of helium lines to the required accuracy, but involving a matrix inversion for 29 energy levels of the helium atom rather than an iterative approach using 3,000 levels. For the calculations proposed here, they use the new, accurate model atom to calculate the radiative transfer for a photoionized nebula. This project involves calculating the recombination cascade for several thousand grid points to provide the requisite accuracy. The group is currently developing the algorithm to carry out the radiative

transfer. They have also obtained a radiative transfer code to check their results.

In addition to radiative transfer calculations, the group has already found that their helium atom model they developed provides a useful input module. However, this routine could be made even more useful if the group was to extend their calculation over a larger range of temperatures and density than done currently. This entails calculating the atomic data ab initio, revising the current fits, and extending several of the tables. This process is computationally intensive, but relatively straightforward.

Research Group

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Paul Woodward, Fellow

Computational Astrophysics

Over the last several years, this research group has been involved in extensive and detailed studies of turbulent convection in stars and of the nature of compressible turbulence in its own right. One project specifically centers on simulations of magnetoconvection using the groupï¿½s new PPM magnetohydrodynamics (MHD) code. The key to this approach is to exploit the extreme parallel nature of the PPM computation on uniform Cartesian grids together with the codeï¿½s very high accuracy and very low effective viscosity. This approach has enabled the group, using very fine grid resolutions, to reach regimes of very low effective viscosity that are essentially unparalleled. The data sets from these simulations contain uniquely detailed information. Most of the groupï¿½s efforts have been put to simulations in which they stir a chunk of gas (with periodic boundary conditions) with a randomly selected set of smooth, well resolved waves, and they then allow the gas to develop turbulence without any further stirring. These calculations demand the greatest grid resolution. Their advantage is that they involve no unphysical continuous stirring mechanisms, and if a self-similar flow develops, as it does, this result cannot be said to have been introduced through the computational approach. This group is extending this work to a more compressible regime and is carrying out such simulations with physical stirring mechanisms such as flow past an obstacle.

This groupï¿½s work on stellar convection and magnetoconvection on uniform Cartesian grids involves very detailed simulation of convection in deep stratified atmospheres with periodic boundary conditions in the horizontal dimensions. This approach is distinguished by its ability to produce turbulent convection flows relatively uncontaminated by thermal effects due to artificial upper surface boundary conditions. This feature of the work enabled these researchers to perform highly detailed statistical comparisons of the simulation results with the predictions of mixing length theories used in computer models of stellar structure and evolution.

Other work is simulating three-dimensional processes in stars. Recently, this groupï¿½s PPM compressible gas dynamics code has been enhanced to enable simulations of hydrodynamical processes in entire three-dimensional model stars. Convection occurs in stars under conditions where the opacity of the gas is too great to allow the heat generated from nuclear reactions in the interior to be transported outward by radiative heat conduction. Convection transports this heat instead by gas motion. Stars like

the sun transport heat by convection in their outer layers. The convective motions carry angular momentum as well as heat, and they act to establish a differential rotation of the star that can be observed for the sun by helioseismology. This differential rotation drives the generation of magnetic fields, which in turn are related to phenomena like sun spots at the stellar surface. This groupï¿½s simulations of the interaction of convection with rotation of a model star in three dimensions allows the group to explore this development of the differential rotation profile in detail for the first time.

This groupï¿½s PPM code has also been adapted to the study of red giant stars. In these stars, convection fills nearly the entire stellar volume so that it is essential to include the global geometry in order to describe the convection properly. Recently, the first full simulation of such a convective envelope was performed, and it revealed the prominence of a global dipole convection mode. In addition, this calculation produced a pulsating envelope apparently stimulated by the violent convection. These new PPM codes are opening up exciting new research areas in stellar astrophysics.

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Studies of the Physics of Quantum Many-Body Systems

The quantum many-body physics program is concerned with the microscopic basis for structure and dynamics of a wide range of many-body systems. All work deals with many degrees of freedom, and most work is ab initio in the sense that it deals with microscopically accurate representations of the systems of interest as opposed to model systems. Generally, many-body physics of strongly correlated systems must make use of large scale computations to be relevant to real physical systems, and the power of present supercomputers is often the chief limiting factor for the research.

This group has developed and is currently applying dynamical Metropolis Monte Carlo simulations to study the approach to equilibrium of the magnetization of magnetic thin films from important initial configurations. The first of these configurations is magnetization orthogonal to the plane of a magnetic film, and the second is the decay of a parallel encoded magnetic bit. In the first, the group has qualitatively reproduced the logarithmic decay of the magnetization of model two-dimensional films. A preliminary report is in preparation, but considerable work is yet to be done in order to apply this to more realistic magnetized films including the fact that they are a finite thickness and that they are composed of magnetic particles of differing sizes, magnetic parameters, and other disordering properties. Similarly, the group has very recent results for the time decay of a magnetic bit encoded through opposing parallel magnetization on a two-dimensional thin filmï¿½a problem of extreme practical interest for archival storage. The researchers have observed a number of different decay modes that must be processed in order to draw even preliminary conclusions. Subsequently, the group must extend this work to more realistic material descriptions and multiple bit decay.

This group is also developing a method of quantum molecular dynamics at finite temperatures applicable to strongly correlated quantum fluids such as the helium liquids and nuclear matter. A time averaging of a pure state density matrix is being implemented with specified energy expectation value E that is not an energy eigenstate. Thus, this method produces a statistical density matrix when averaged over a long enough time. However, it does not satisfy the maximum entropy principle when beginning with an arbitrary state, and the group chooses the initial state to approximately maximize the entropy of the resulting density matrix. It appears that large scale multi-processor computation is necessary to carry out the time evolution and averaging as well as to evaluate the entropy. This method can be improved in principle by beginning with a density matrix for which the entropy has already been approximately maximized, but this is more numerically cumbersome and is deferred to future work.

This group is also continuing a project on the scattering of boson particles from superfluid boson slabs

and clusters where the scattered particle is identical to the particles that make up the scattering fluid. The cluster work is focused on a weakly, repulsively interacting Bose gas confined by a spherical potential well with parameters chosen to represent the experimental work underway on Bose condensed Rb clusters. The slab work is on scattering helium-4 atoms from a superfluid helium-4 slab. This helium work requires massive variational Monte Carlo simulations. These researchers have completed and published the pure condensate mediated part of the helium work and are now investigating the competing processes of elementary excitation mediated transmission and scattering in order to see if the relative intensity of the former survives the competition of the latter at a measurable level.

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Cynthia A. Cattell, Associate Fellow

Kinetic Physics of the Magnetotail and Auroral Zone

The auroral acceleration region is characterized by regions of alternating upward and downward current. The commonly held view of the source of particle acceleration is a quasistatic electric field with a component parallel to the Earthï¿½s magnetic field and extended for hundreds to thousands of kilometers. Ionospheric ion species enter the acceleration and are accelerated upward, each species gaining a different average drift because of their different mass. The relative drift is the free energy source for a two-stream instability. Both electron beams and currents can also excite electrostatic waves. An outstanding question is identification of the source of free energy for particularly observed electrostatic waves. The particular species that supply the free energy has implications for heating mechanisms for various particle populations, the formation of nonlinear waveforms, and the viability of suggested mechanisms for forming electric potential structures that produce aurora. This group has analyzed the linear stability of two upflowing ion events and two upward streaming electron events from new Fast Auroral Snapshot (FAST) satellite auroral zone data. The investigation proceeds with the study of further events and with more careful analysis and fitting of the model to the observed distribution functions. While the bi-Maxwellian model is fairly adequate for modeling populations in the upward current region, the electrons in the downward current region are not Maxwellian. Rather, they carry a heat flux up the magnetic field line. They appear as bi-Maxwellians with very low perpendicular compared to parallel temperatures. A new theoretical model of this distribution named

Tri-Maxwellian has been developed and is being included in the stability code. The group is using the data to determine the drift velocity, density, and three temperatures that will be used for this model distribution and then determine the stability of upflowing electrons with greater accuracy.

To address the question of the effect of perturbation electric and magnetic fields on energization, scattering, and transport of charged particles in field-reversed magnetic field geometries, this group has utilized numerical codes to trace the trajectories in specific prescribed background magnetic fields for several different types of perturbations. Their research is focused in two areasï¿½the effects of low frequency electrostatic waves on energization, transport, and the classification of orbits of ions in the Earthï¿½s magnetotail and on the effects of ultra-low frequency (ULF) electromagnetic waves on transport, energization, and scattering of ions in the magnetosphere of Neptune. This groupï¿½s preliminary studies indicate observations can dramatically change the trajectories of particles. Recent work has provided information on the energization of particles and changes in distribution functions. Because of the broad range of critical question in the physics of the magnetosphere that researchers have answered on the basis of trajectory studies that neglect perturbations, it is vital to determine whether the inclusion of realistic perturbations invalidates the conclusions.

This group is performing test particle calculations using models appropriate to the specific planetary magnetosphere being studied. They have added diagnostics to determine bulk energization and pitch angle scattering, modeling of distributions, and pseudo-surface of section plots. Studies of processes occurring in the magnetospheres of the outer planets has provided a unique opportunity to extend the understanding of space plasma physics. Understanding which processes associated with the motion of particles in a field-reversed magnetic field are important in all planetary magnetospheres and their similarities and differences can help apply results to astrophysical systems different from the Earth.

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J. Woods Halley, Fellow

Numerical Studies of Fluids and Disordered Solids

Traditional theoretical models of electrode-electrolyte interfaces give qualitative insight at best. This discussion is divided into three parts by this groupï¿½studies of outer shell electron transfer rates at metal electrodes, studies of inner shell processes at metal electrodes, and studies of semiconductor-water interfaces of interest in photoelectrochemistry and corrosion.

This group has obtained results on the cuprous-cupric electron transfer reaction in water at a copper electrode. The copper electron transfer reaction differs from previous study; electrode approach energy dominates the reaction barrier. Improvements in techniques and analysis developed during the cuprous-cupric and ferrous-ferric electron transfer studies are currently being implemented. The group is also

modeling electrolyte screening of the electric field in their simulations of the cuprous-cupric electron transfer. For inner shell processes, simultaneous calculation of metallic electronic structure and atomic dynamics is required. The wave function for the electrons associated with the metal electrode are recomputed at each step in the molecular dynamics simulation. Water is treated classically, but interaction of water with electrons of the metal are taken into account with a pseudopotential. For semiconductor-water interfaces, work has been extended to include atomic motion and make calculations Hartree self-consistent. The group is currently studying localized electronic states (polarons) in bulk rutile as a function of temperature and box size using this code. They have preliminary results that demonstrate that localization occurs at temperatures below 100 K. This code is used to study the dissociation of water at the surface and the transport of ions through such an oxide in environments that model the behavior of passivation layers protecting titanium metal from corrosion.

In a study of transport of ions in polymers with battery applications in view, the group focused on molecular dynamics and Monte Carlo calculations of Li+ and various anions in glassy polymers in order to study transport and ion pairing. Recently, the neutron scattering collaborations have produced experimental data on the structure of molten polyethylene oxide with results in good agreement with the model. To study transport in the polymer system, ab initio potentials are being used to obtain the frequency dependence of the conductivity by direct simulation. For the lithium perchlorate system in polyethylene oxide, the studies have been extended to higher ionic concentrations characteristic of battery applications and are currently being completed. The group has been carrying out a study of ion pairing in the lithium perchlorate/polyethylene oxide system as well and have obtained results that confirm the hypothesis that ion pairing in the lithium perchlorate system is entropically driven.

These researchers are also engaged in a theoretical and computational analysis of a novel method for the detection of the Boson condensate in superfluid helium four. Helium atoms incident on a superfluid in a finite geometry are expected to be transmitted by a condensate mediated process (CMP). Using a Quantum Variational Monte Carlo approach, the researchers have obtained results for the transmission times that are consistent with earlier perturbation theory and uncertainty principle estimates. The next step is the inclusion of phonon/roton/ripplon processes into the analysis. The researchers optimize a variational wavefunction subject to the constraints of energy and probability current conservation. Incorporating the phonon/roton/ripplon processes requires more complex searches over a larger phase space than was used in the analysis for the CMP alone. A similar analysis has been carried out for atomic scattering from Bose-Einstein condensed dilute alkali vapors.

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Kinetic Physics of the Magnetotail and Auroral Zone

These researchers are continuing to analyze data from their experiments at the Los Alamos Meson Physics Facility (LAMPF) and the Indiana University Cyclotron Facility (IUCF) on nuclear structure with intermediate energy protons. The experiments are followed by a detailed numerical analysis of the data to compare these researchers results with current models of the fundamental proton-nucleus interaction and nuclear structure. For this purpose, the group has developed, or modified, a number of large computer codes for use on the supercomputers.

Currently, there are three areas in which the researchers have final data requiring analysis. These areas include measurements of elastic and inelastic proton cross sections and spin observables at several energies, scattering measurements on non-spherical nuclei to determine nuclear size and shape parameters, and two neutron pickup reactions to measure pairing correlations in nuclei.

In the first case, the primary interest is in the modification of the fundamental proton-proton and neutron interactions inside of the nuclear medium. This nuclear density dependence is fundamental to the theory of proton-nucleus interactions and is of direct significance to astrophysical theories on the origin of the universe and the dynamics of neutron stars and black holes. The modification of the nucleon-nucleon interaction in nuclei is a manifestation of the underlying quark structure of nucleons.

In the second area, determination of the nuclear shape parameters (quadruple, octuple, hexadecapule,

and higher) are compared with modern Boson models for nuclear excitation modes.

In the last area, the experiments are very sensitive to the departures of the motion of individual nucleons in the nucleus from completely independent orbits (pairing correlations are the most important). The experiments can also give, upon analysis, information on the modifications discussed above of the nucleon-nucleon interaction when the nucleons interact in states of high angular momentum.

Research Group

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Numerical Investigations of Solar Wind-Magnetosphere-Ionosphere Coupling

The main goal of this research is to understand solar wind-magnetosphere-ionosphere coupling (i.e., the transfer of the mass, momentum, and energy of the solar wind through the earthï¿½s magnetosphere and to the ionosphere) and the implications of this coupling for the formation of the aurora. The solar wind impinges on the magnetospheric boundary, which is known as the magnetopause. On the front side of the magnetopause, the solar wind velocity is normal to the magnetopause surface, and variations in the solar wind dynamic pressure can cause fluctuations in the magnetopause position. This part of the boundary is susceptible to the magnetohydrodynamics (MHD) version of the Rayleigh-Taylor instability. As one moves toward the dawn or dusk flanks of the magnetopause, the solar wind velocity becomes tangential to the magnetopause, and the resulting shear flow is susceptible to the Kelvin-Helmholtz instability. In the intermediate region, both instabilities may be operative. This group is currently extending this model to three dimensions, allowing for a more realistic description of the coupling of the outer magnetosphere to the ionosphere. Previous work in this area has used a two-dimensional, incompressible, spectral code. The difficulty here is that the evolution of these instabilities is on a time scale comparable to the transit time of Alfvï¿½n waves between the magnetosphere and ionosphere. Properly including this Alfvï¿½n wave propagation requires a three-dimensional model.

Once energy is transported into the magnetosphere, it is carried to the inner magnetosphere and ionosphere by the propagation of shear mode Alfvï¿½n waves that propagate along the magnetic field and carry field-aligned current. The presence of Alfvï¿½n waves in the auroral zone can be observed from the ground by magnetometer arrays that detect the magnetic perturbations of these waves. The theory of the production of these ground signatures is well established for long period waves, but it is more complicated for the waves near one second period associated with the aurora. This group has developed a two-dimensional MHD code to describe this propagation. With this code, they have determined the effects of the atmosphere at modifying the Alfvï¿½n wave signature as observed on this ground. The first version of this code considered a system that was homogeneous in the horizontal direction, an assumption that fails in the auroral zone where density cavities confined in the horizontal direction are observed. The researchers have developed a model to include such horizontal inhomogeneities in a simplified version of the code, and this is being extended to the full code. In addition, they are extending the model to three dimensions to more realistically model the ground

signatures of localized current distributions.

The final project involves the acceleration of electrons in Alfvï¿½n waves, and this model is extended to treat ions. The ion calculation is complicated by the fact that while the electrons can be treated in the guiding center approximation, the full ion dynamics must be included since the Alfvï¿½n waves can have perpendicular wavelengths that are small compared to the ion gyroradius. These test particle models can produce non-Maxwellian particle distribution in the electrons and ions. By combining these codes, the group is able to provide more complete predictions for the particle and wave measurements made along auroral field lines. These predictions are then compared with results from the recently launched Polar and Fast Auroral Snapshot (FAST) satellites.

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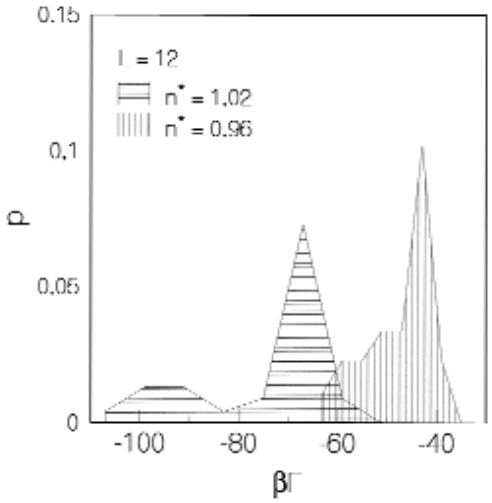
Numerical Studies in Condensed Matter Theory

This group is continuing their study of the properties of superconductors with unconventional pairing states. In one project, the researchers are using the numerical methods they have developed to solve the nonlinear London equations to compute the magnetic penetration depth as a function of the angle between crystallographic axes and applied magnetic field. In a second task, they are using numerical Renormalization Group methods to study finite size effects in the normal to superconductor phase transition in layered superconductors. A third task being undertaken is the calculation of the tunneling spectra in junctions between a ferromagnet and an unconventional superconductor. In a fourth task, the group is studying transport properties of layered superconductors along the crystallographic c-axis. In addition to high-temperature superconductors, this group is emphasizing other materials in which evidence for unconventional superconductivity has been accumulating. These include heavy fermion compounds, organic salt superconductors, and certain cubic perovskites to name a few.

Further work is being done on the microcanonical Monte Carlo method developed by this group. This method has made computational efficiency of simulations considerably better than that of conventional Monte Carlo procedures. This method is being used and extended to continue the study of the topography of the phase space (the structure of metastable minima separated by local maxima) of a glassy system. The current emphasis is on the inclusion of the effects of defects and impurities through the introduction of a random potential in the simulation. As a new task in this area, the group is beginning a study of freezing. They plan to develop their ideas in terms of general considerations applicable to the freezing transition in systems such as liquid crystals that exhibit a succession of phases.



Density of states for glassy free energy minima obtained from a novel Monte Carlo procedure to study the free energy landscape of a glassy hard sphere system. Results at two densities are shown. (To appear in Physical Review E).

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Thomas F. Walsh, Fellow

Lattice Studies of the Gluon Propagator

These researchers are studying the gluon propagator on large lattices. The lattices from which the propagators are calculated can also be used to calculate hadron properties and are generated using full quantum chromodynamics (QCD) with Kogut-Susskind fermions. These researchers use the Hybrid Monte Carlo method that makes use of molecular dynamics techniques. Their techniques and numerical methods are of interest to many researchers seeking to optimize similarly complicated algorithms on MPP systems and on the Cray T3D supercomputer in particular.

Research Group

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Theoretical Physics Institute

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Leonid Glazman
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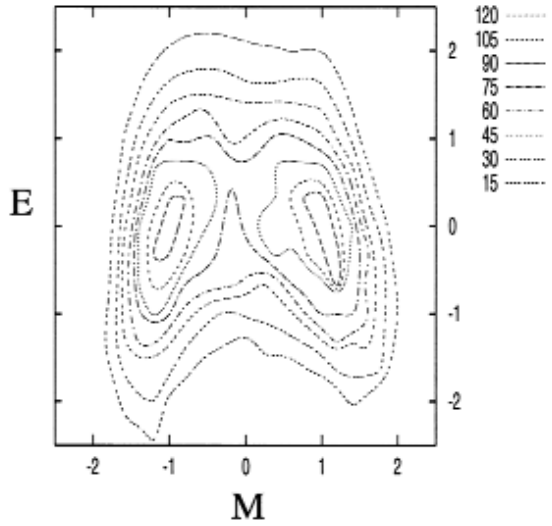
Philippe de Forcrand, Fellow

The Deconfinement Phase Transition in One-Flavor Quantum Chromodynamics

These researchers studied the deconfinement phase transition of one-flavor Quantum Chromodynamics (QCD) using the multiboson algorithm. The mass of the Wilson fermions relevant for this study is moderately large, and the non-hermitian multiboson method is a superior simulation algorithm. Finite size scaling is studied on lattices of size 83 X 4, 123 X 4, and 163 X 4. The behaviors of the peak of the Polyakov loop susceptibility, the deconfinement ratio, and the distribution of the norm of the Polyakov loop are all characteristic of a first-order phase transition for heavy quarks. As the quark mass decreases, the first-order transition gets weaker and turns into a crossover. To investigate finite size scaling on larger spatial lattices, these researchers use an effective action in the same universality class as QCD. This effective action is constructed by replacing the fermionic determinant with the Polyakov loop identified as the most relevant Z(3) symmetry breaking term. Higher-order effects are incorporated in an effective Z(3)-breaking field, h, which couples to the Polyakov loop. Finite size scaling determines the value of h where the first order transition ends. This analysis, at the endpoint hep, indicates that the effective model and QCD are consistent with the universality class of the three-dimensional Ising model. Matching the field strength at the end point hep to the k values used in the dynamical quark simulations, the group estimated the endpoint hep of the first-order phase transition. They found hep ~ 0.08, which corresponds to a quark mass of about 1.4 GeV.



Distribution of the magnetization M and energy E at the second-order endpoint of the deconfinement transition line.

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Leonid Glazman, Principal Investigator

Monte-Carlo study of Vortex Phase Diagram in Layered Superconductors

Thermodynamics and transport properties of Type II superconductors in magnetic field are essentially properties of the "vortex matter." A peculiarity of high Tc superconductors is a very high amplitude of thermal fluctuations in the vortex state. This leads to destruction of the low-temperature vortex crystal state well below the mean field upper critical field. The only way to obtain quantitative information about the phase diagram in the vortex state is large-scale numerical simulations.

The researchers at the Theoretical Physics Institute have used time provided by the Supercomputing Institute to study the phase diagram by Monte-Carlo simulations of the three-dimensional, uniformly frustrated XY model. They have investigated the properties of the melting transition for different anisotropy parameters. The study shows that the pancake alignment above the melting transition increases with decreasing of the anisotropy. At high anisotropies, the melting is accompanied by a significant drop in the coupling energy and the destruction of vortex lines, while at small anisotropies the vortex lines preserve their continuity at the melting transition. In the linelike melting regime, the researchers find several universal properties of the transition and of the liquid phase. These properties include the scaling of the melting temperature with anisotropy and magnetic field, the effective line tension of vortices in the liquid regime, the latent heat, the entropy jump per entanglement length, and relative jump of Josephson energy at the transition as compared to the latent heat. Simulations advanced understanding of the vortex phase diagram in layered high-temperature superconductors.
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Larry McLerran, Principal Investigator

Improved Actions for Quantum Chromodynamics on Anisotropic Lattices

To achieve accurate results from lattice Quantum Chromodynamics (QCD), it is necessary to improve the lattice actions used in simulations. In the Symanzik improvement program, which this group is pursuing, one adds higher dimensional operators to the action (and currents) to eliminate the leading discretization errors affecting rotational or chiral symmetry. The so-called Schrodinger functional has recently become a powerful tool in eliminating the O(a) errors (a = lattice spacing) violating chiral symmetry non-perturbatively in the coupling. This tool is helping to eliminate the O(a) errors of quark actions on anisotropic lattices. This finally allows accurate simulations of heavy quarks.

As a first step in carrying out the program of QCD on anisotropic lattices (with spatial spacing a_s and temporal spacing a_t) with improved actions, the Schrodinger functional method was used to determine the renormalization of the anisotropy (a_s / a_t). This involves Monte Carlo measurements at various anisotropies as well as various gauge couplings (related to the lattice spacings).

Previous work has generated approximately 350 configurations at bare anisotropy 2 and only 20 configurations for thermalization of the system at anisotropy 4. This has been done for only one value of the coupling (beta) corresponding to a moderately coarse lattice. In order to achieve accurate statistics, at least 500 configurations are needed for each anisotropy at each coupling. These configurations are used for purposes beyond understanding the renormalized anisotropy. The same configurations are used in the improvement of the quark action on anisotropic lattices, which leads to accurate simulation of heavy quark systems.
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School of Physics and Astronomy

Department of Astronomy

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Evan D. Skillman
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Thomas W. Jones, Fellow

Numerical Studies of Particles and Fluids in Astrophysics

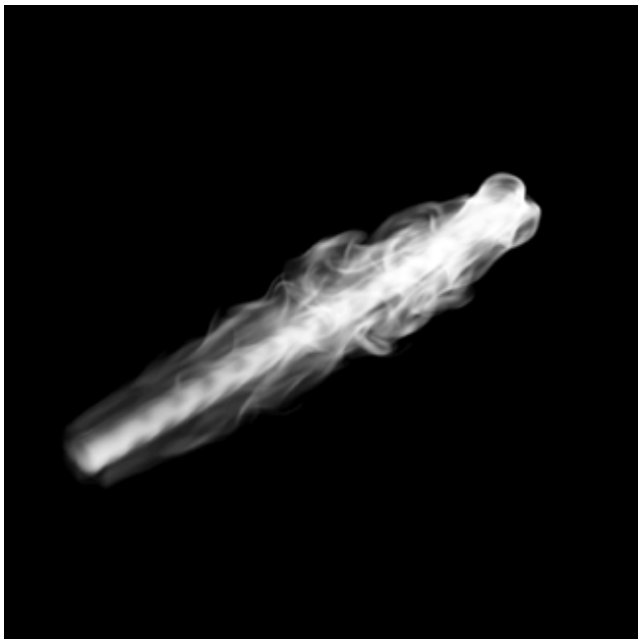
This research continues a very successful pioneering program in computational astrophysics. The program is centered on improving the fundamental understanding of the behaviors of high-energy charged particles (also known as Cosmic-Rays) and magnetic fields in cosmic plasmas and the application of this knowledge to the understanding of some recognized key astrophysical problems; namely, the origins of the cosmic-rays, the nature of giant radio galaxies, the nature of supernova remnants, and the nature of the interstellar medium in our galaxy. The specific work under current progress is carrying out two significant simulations based on state-of-the-art codes for compressible magnetohydrodynamics (MHD) and novel schemes for following the acceleration and propagation of cosmic-rays.

The first part of the work involves carrying out the first three-dimensional MHD simulations of particle transport and radiation from radio galaxies. These simulations include the acceleration and transport of the relativistic electrons producing the observed emission. This is an extension of the two-dimensional MHD simulations already completed. This is an important step that allows, for the first time, modeling a direct connection between the flow dynamics of the jets driving the phenomenon and observed properties of the objects. These are the first calculations that allow a real test of the basic hypotheses

used in the field. The extension to three dimensions is important because it allows the researchers to drop the limiting assumption of axis-symmetry in the jet flow and allows for the proper full development of three-dimensional turbulence in the magnetized back-flow of the jet material. This is the primary region of radio emission, and the emission is highly sensitive to the strength and structure of the magnetic fields. The group is currently carrying out a high resolution simulation on a 3842 X 768 grid. The calculations need to be continued for at least twenty dynamical times. Because of the very complex dynamics in these flows, and the importance of capturing that for proper determination of the magnetic field evolution, it is important to include simulations of the highest spatial resolution possible. The simulations include momentum dependence to the relativistic electrons so they are effectively four-dimensional.

The other part of the work centers on three-dimensional MHD simulations of supersonic cosmic plasma clouds. This group has carried out the first two-dimensional MHD simulations of the evolution of supersonic gas clouds in the interstellar medium, and more recently completed a detailed study of collisions between such clouds. Statistically, such collisions are supposed to happen about once in a million years. This groupï¿½s studies have shown that if magnetic fields are absent, these clouds are largely disrupted individually. However, they found that even a modest magnetic field can be a very important stabilizing influence. In fact, in two-dimensional simulations, the field may effectively shield the clouds from almost any dynamical destruction. If this is really valid, it has profound implications for the structure of the interstellar medium where there is a small but significant magnetic field. This work is being extended to three-dimensional flows using the codes developed by this group. Only in this way can they establish the importance of the two-dimensional symmetry assumed in earlier computations. The group has speculated that if clouds have a roughly spherical shape, magnetic fields may be largely shed, but a sausage shaped cloud may be able to hold onto the local field to build it into a shield. Currently, the group is carrying out high resolution three-dimensional MHD simulations of interstellar clouds.

The third area of recent effort has been development of new computational tools for the simulation of particle transport and acceleration near shocks. Accurate treatment with realistic parameters is technically very challenging, since it requires spatial resolutions ranging over several orders of magnitude from the physical thickness of the shocks. The group is introducing, for the first time, adaptive mesh refinement techniques and sub-zone shock tracking into this problem. This will also enable a more physically complete treatment of the injection of nonthermal particles from the thermal plasma population at shocks. Early results are very promising.



Synthetic radio emission image of a simulated cosmic hypersonic plasma jet. The three-dimensional magnetohydrodynamics simulation was the first of its kind to include explicit transport of high-energy electrons that produce the observed radio emission in cosmic "radio jets."

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Steps to the Primordial Helium Abundance

The value of the primordial helium abundance, the fraction of baryonic matter converted to helium in nucleosynthesis shortly after the Big Bang, is an extremely important constraint on current cosmological models. The amount of helium created constrains the total mass density and rate of expansion of the Universe. An upper limit on this value comes from measuring the helium abundance in emission line nebulae of metal poor dwarf galaxies. Such galaxies, with a gas reservoir relatively unpolluted with the nucleosynthetic products of stars, yield the lowest known helium abundances.

Since the variation of helium abundance with cosmological parameters is small, it is important to constrain this value to within one percent or so. Since the brighter helium emission lines in these galaxies can now be measured with an accuracy of this level, it remains to be determined whether the steps required to convert these emission lines to abundances are also secure to within one percent and to limit the systematic uncertainties. To this end, this group has carried out the most accurate calculation to date of the helium emission spectrum, including several improvements in the atomic data over previous calculations. In addition, this group has attached an uncertainty to the predicted emissivities for the first time based on assessment of the quality of the input atomic data.

The group then compared the results of their calculations to the observed helium emission spectra in three nebulae. While their calculations yielded better agreement with the data than previous work, there still remained several discrepant lines. Some of these discrepancies are almost certainly due to radiative transfer effects; absorption of nebular photons by the helium atoms in a metastable state alters the recombination cascade and the resulting intensities.

This group has developed fitting functions to the atomic data that allow them to calculate the emissivity of helium lines to the required accuracy, but involving a matrix inversion for 29 energy levels of the helium atom rather than an iterative approach using 3,000 levels. For the calculations proposed here, they use the new, accurate model atom to calculate the radiative transfer for a photoionized nebula. This project involves calculating the recombination cascade for several thousand grid points to provide the requisite accuracy. The group is currently developing the algorithm to carry out the radiative transfer. They have also obtained a radiative transfer code to check their results.

In addition to radiative transfer calculations, the group has already found that their helium atom model they developed provides a useful input module. However, this routine could be made even more useful if the group was to extend their calculation over a larger range of temperatures and density than done currently. This entails calculating the atomic data ab initio, revising the current fits, and extending several of the tables. This process is computationally intensive, but relatively straightforward.

Research Group

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Paul Woodward, Fellow

Computational Astrophysics

Over the last several years, this research group has been involved in extensive and detailed studies of turbulent convection in stars and of the nature of compressible turbulence in its own right. One project specifically centers on simulations of magnetoconvection using the groupï¿½s new PPM magnetohydrodynamics (MHD) code. The key to this approach is to exploit the extreme parallel nature of the PPM computation on uniform Cartesian grids together with the codeï¿½s very high accuracy and very low effective viscosity. This approach has enabled the group, using very fine grid resolutions, to reach regimes of very low effective viscosity that are essentially unparalleled. The data sets from these simulations contain uniquely detailed information. Most of the groupï¿½s efforts have been put to simulations in which they stir a chunk of gas (with periodic boundary conditions) with a randomly selected set of smooth, well resolved waves, and they then allow the gas to develop turbulence without any further stirring. These calculations demand the greatest grid resolution. Their advantage is that they involve no unphysical continuous stirring mechanisms, and if a self-similar flow develops, as it does, this result cannot be said to have been introduced through the computational approach. This group is extending this work to a more compressible regime and is carrying out such simulations with physical stirring mechanisms such as flow past an obstacle.

This groupï¿½s work on stellar convection and magnetoconvection on uniform Cartesian grids involves very detailed simulation of convection in deep stratified atmospheres with periodic boundary conditions in the horizontal dimensions. This approach is distinguished by its ability to produce turbulent convection flows relatively uncontaminated by thermal effects due to artificial upper surface boundary conditions. This feature of the work enabled these researchers to perform highly detailed statistical comparisons of the simulation results with the predictions of mixing length theories used in computer models of stellar structure and evolution.

Other work is simulating three-dimensional processes in stars. Recently, this groupï¿½s PPM compressible gas dynamics code has been enhanced to enable simulations of hydrodynamical processes in entire three-dimensional model stars. Convection occurs in stars under conditions where the opacity of the gas is too great to allow the heat generated from nuclear reactions in the interior to be transported outward by radiative heat conduction. Convection transports this heat instead by gas motion. Stars like the sun transport heat by convection in their outer layers. The convective motions carry angular momentum as well as heat, and they act to establish a differential rotation of the star that can be observed for the sun by helioseismology. This differential rotation drives the generation of magnetic fields, which in turn are related to phenomena like sun spots at the stellar surface. This groupï¿½s simulations of the interaction of convection with rotation of a model star in three dimensions allows the group to explore this development of the differential rotation profile in detail for the first time.

This groupï¿½s PPM code has also been adapted to the study of red giant stars. In these stars, convection fills nearly the entire stellar volume so that it is essential to include the global geometry in order to describe the convection properly. Recently, the first full simulation of such a convective envelope was performed, and it revealed the prominence of a global dipole convection mode. In addition, this calculation produced a pulsating envelope apparently stimulated by the violent convection. These new PPM codes are opening up exciting new research areas in stellar astrophysics.

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Studies of the Physics of Quantum Many-Body Systems

The quantum many-body physics program is concerned with the microscopic basis for structure and

dynamics of a wide range of many-body systems. All work deals with many degrees of freedom, and most work is ab initio in the sense that it deals with microscopically accurate representations of the systems of interest as opposed to model systems. Generally, many-body physics of strongly correlated systems must make use of large scale computations to be relevant to real physical systems, and the power of present supercomputers is often the chief limiting factor for the research.

This group has developed and is currently applying dynamical Metropolis Monte Carlo simulations to study the approach to equilibrium of the magnetization of magnetic thin films from important initial configurations. The first of these configurations is magnetization orthogonal to the plane of a magnetic film, and the second is the decay of a parallel encoded magnetic bit. In the first, the group has qualitatively reproduced the logarithmic decay of the magnetization of model two-dimensional films. A preliminary report is in preparation, but considerable work is yet to be done in order to apply this to more realistic magnetized films including the fact that they are a finite thickness and that they are composed of magnetic particles of differing sizes, magnetic parameters, and other disordering properties. Similarly, the group has very recent results for the time decay of a magnetic bit encoded through opposing parallel magnetization on a two-dimensional thin filmï¿½a problem of extreme practical interest for archival storage. The researchers have observed a number of different decay modes that must be processed in order to draw even preliminary conclusions. Subsequently, the group must extend this work to more realistic material descriptions and multiple bit decay.

This group is also developing a method of quantum molecular dynamics at finite temperatures applicable to strongly correlated quantum fluids such as the helium liquids and nuclear matter. A time averaging of a pure state density matrix is being implemented with specified energy expectation value E that is not an energy eigenstate. Thus, this method produces a statistical density matrix when averaged over a long enough time. However, it does not satisfy the maximum entropy principle when beginning with an arbitrary state, and the group chooses the initial state to approximately maximize the entropy of the resulting density matrix. It appears that large scale multi-processor computation is necessary to carry out the time evolution and averaging as well as to evaluate the entropy. This method can be improved in principle by beginning with a density matrix for which the entropy has already been approximately maximized, but this is more numerically cumbersome and is deferred to future work.

This group is also continuing a project on the scattering of boson particles from superfluid boson slabs and clusters where the scattered particle is identical to the particles that make up the scattering fluid. The cluster work is focused on a weakly, repulsively interacting Bose gas confined by a spherical potential well with parameters chosen to represent the experimental work underway on Bose condensed Rb clusters. The slab work is on scattering helium-4 atoms from a superfluid helium-4 slab. This helium work requires massive variational Monte Carlo simulations. These researchers have completed and published the pure condensate mediated part of the helium work and are now investigating the competing processes of elementary excitation mediated transmission and scattering in order to see if the relative intensity of the former survives the competition of the latter at a measurable level.

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Cynthia A. Cattell, Associate Fellow

Kinetic Physics of the Magnetotail and Auroral Zone

The auroral acceleration region is characterized by regions of alternating upward and downward current. The commonly held view of the source of particle acceleration is a quasistatic electric field with a component parallel to the Earthï¿½s magnetic field and extended for hundreds to thousands of kilometers. Ionospheric ion species enter the acceleration and are accelerated upward, each species gaining a different average drift because of their different mass. The relative drift is the free energy source for a two-stream instability. Both electron beams and currents can also excite electrostatic waves. An outstanding question is identification of the source of free energy for particularly observed electrostatic waves. The particular species that supply the free energy has implications for heating mechanisms for various particle populations, the formation of nonlinear waveforms, and the viability of suggested mechanisms for forming electric potential structures that produce aurora. This group has analyzed the linear stability of two upflowing ion events and two upward streaming electron events from new Fast Auroral Snapshot (FAST) satellite auroral zone data. The investigation proceeds with the study of further events and with more careful analysis and fitting of the model to the observed distribution functions. While the bi-Maxwellian model is fairly adequate for modeling populations in the upward current region, the electrons in the downward current region are not Maxwellian. Rather, they carry a heat flux up the magnetic field line. They appear as bi-Maxwellians with very low perpendicular compared to parallel temperatures. A new theoretical model of this distribution named Tri-Maxwellian has been developed and is being included in the stability code. The group is using the data to determine the drift velocity, density, and three temperatures that will be used for this model distribution and then determine the stability of upflowing electrons with greater accuracy.

To address the question of the effect of perturbation electric and magnetic fields on energization, scattering, and transport of charged particles in field-reversed magnetic field geometries, this group has utilized numerical codes to trace the trajectories in specific prescribed background magnetic fields for several different types of perturbations. Their research is focused in two areasï¿½the effects of low frequency electrostatic waves on energization, transport, and the classification of orbits of ions in the Earthï¿½s magnetotail and on the effects of ultra-low frequency (ULF) electromagnetic waves on transport, energization, and scattering of ions in the magnetosphere of Neptune. This groupï¿½s preliminary studies indicate observations can dramatically change the trajectories of particles. Recent work has provided information on the energization of particles and changes in distribution functions. Because of the broad range of critical question in the physics of the magnetosphere that researchers have answered on the basis of trajectory studies that neglect perturbations, it is vital to determine whether the inclusion of realistic perturbations invalidates the conclusions.

This group is performing test particle calculations using models appropriate to the specific planetary magnetosphere being studied. They have added diagnostics to determine bulk energization and pitch angle scattering, modeling of distributions, and pseudo-surface of section plots. Studies of processes occurring in the magnetospheres of the outer planets has provided a unique opportunity to extend the understanding of space plasma physics. Understanding which processes associated with the motion of particles in a field-reversed magnetic field are important in all planetary magnetospheres and their similarities and differences can help apply results to astrophysical systems different from the Earth.

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J. Woods Halley, Fellow

Numerical Studies of Fluids and Disordered Solids

Traditional theoretical models of electrode-electrolyte interfaces give qualitative insight at best. This discussion is divided into three parts by this groupï¿½studies of outer shell electron transfer rates at metal electrodes, studies of inner shell processes at metal electrodes, and studies of semiconductor-water interfaces of interest in photoelectrochemistry and corrosion.

This group has obtained results on the cuprous-cupric electron transfer reaction in water at a copper electrode. The copper electron transfer reaction differs from previous study; electrode approach energy dominates the reaction barrier. Improvements in techniques and analysis developed during the cuprous-cupric and ferrous-ferric electron transfer studies are currently being implemented. The group is also modeling electrolyte screening of the electric field in their simulations of the cuprous-cupric electron transfer. For inner shell processes, simultaneous calculation of metallic electronic structure and atomic dynamics is required. The wave function for the electrons associated with the metal electrode are recomputed at each step in the molecular dynamics simulation. Water is treated classically, but interaction of water with electrons of the metal are taken into account with a pseudopotential. For semiconductor-water interfaces, work has been extended to include atomic motion and make calculations Hartree self-consistent. The group is currently studying localized electronic states (polarons) in bulk rutile as a function of temperature and box size using this code. They have preliminary results that demonstrate that localization occurs at temperatures below 100 K. This code is used to study the dissociation of water at the surface and the transport of ions through such an oxide in environments that model the behavior of passivation layers protecting titanium metal from corrosion.

In a study of transport of ions in polymers with battery applications in view, the group focused on molecular dynamics and Monte Carlo calculations of Li+ and various anions in glassy polymers in order to study transport and ion pairing. Recently, the neutron scattering collaborations have produced experimental data on the structure of molten polyethylene oxide with results in good agreement with the model. To study transport in the polymer system, ab initio potentials are being used to obtain the

frequency dependence of the conductivity by direct simulation. For the lithium perchlorate system in polyethylene oxide, the studies have been extended to higher ionic concentrations characteristic of battery applications and are currently being completed. The group has been carrying out a study of ion pairing in the lithium perchlorate/polyethylene oxide system as well and have obtained results that confirm the hypothesis that ion pairing in the lithium perchlorate system is entropically driven.

These researchers are also engaged in a theoretical and computational analysis of a novel method for the detection of the Boson condensate in superfluid helium four. Helium atoms incident on a superfluid in a finite geometry are expected to be transmitted by a condensate mediated process (CMP). Using a Quantum Variational Monte Carlo approach, the researchers have obtained results for the transmission times that are consistent with earlier perturbation theory and uncertainty principle estimates. The next step is the inclusion of phonon/roton/ripplon processes into the analysis. The researchers optimize a variational wavefunction subject to the constraints of energy and probability current conservation. Incorporating the phonon/roton/ripplon processes requires more complex searches over a larger phase space than was used in the analysis for the CMP alone. A similar analysis has been carried out for atomic scattering from Bose-Einstein condensed dilute alkali vapors.

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Kinetic Physics of the Magnetotail and Auroral Zone

These researchers are continuing to analyze data from their experiments at the Los Alamos Meson Physics Facility (LAMPF) and the Indiana University Cyclotron Facility (IUCF) on nuclear structure with intermediate energy protons. The experiments are followed by a detailed numerical analysis of the data to compare these researchers results with current models of the fundamental proton-nucleus interaction and nuclear structure. For this purpose, the group has developed, or modified, a number of large computer codes for use on the supercomputers.

Currently, there are three areas in which the researchers have final data requiring analysis. These areas include measurements of elastic and inelastic proton cross sections and spin observables at several energies, scattering measurements on non-spherical nuclei to determine nuclear size and shape parameters, and two neutron pickup reactions to measure pairing correlations in nuclei.

In the first case, the primary interest is in the modification of the fundamental proton-proton and neutron interactions inside of the nuclear medium. This nuclear density dependence is fundamental to the theory of proton-nucleus interactions and is of direct significance to astrophysical theories on the origin of the universe and the dynamics of neutron stars and black holes. The modification of the nucleon-nucleon interaction in nuclei is a manifestation of the underlying quark structure of nucleons.

In the second area, determination of the nuclear shape parameters (quadruple, octuple, hexadecapule, and higher) are compared with modern Boson models for nuclear excitation modes.

In the last area, the experiments are very sensitive to the departures of the motion of individual nucleons in the nucleus from completely independent orbits (pairing correlations are the most important). The experiments can also give, upon analysis, information on the modifications discussed above of the nucleon-nucleon interaction when the nucleons interact in states of high angular momentum.

Research Group

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Numerical Investigations of Solar Wind-Magnetosphere-Ionosphere Coupling

The main goal of this research is to understand solar wind-magnetosphere-ionosphere coupling (i.e., the transfer of the mass, momentum, and energy of the solar wind through the earthï¿½s magnetosphere and to the ionosphere) and the implications of this coupling for the formation of the aurora. The solar wind impinges on the magnetospheric boundary, which is known as the magnetopause. On the front side of the magnetopause, the solar wind velocity is normal to the magnetopause surface, and variations in the solar wind dynamic pressure can cause fluctuations in the magnetopause position. This part of the boundary is susceptible to the magnetohydrodynamics (MHD) version of the Rayleigh-Taylor instability. As one moves toward the dawn or dusk flanks of the magnetopause, the solar wind velocity becomes tangential to the magnetopause, and the resulting shear flow is susceptible to the Kelvin-Helmholtz instability. In the intermediate region, both instabilities may be operative. This group is currently extending this model to three dimensions, allowing for a more realistic description of the coupling of the outer magnetosphere to the ionosphere. Previous work in this area has used a two-dimensional, incompressible, spectral code. The difficulty here is that the evolution of these instabilities is on a time scale comparable to the transit time of Alfvï¿½n waves between the magnetosphere and ionosphere. Properly including this Alfvï¿½n wave propagation requires a three-dimensional model.

Once energy is transported into the magnetosphere, it is carried to the inner magnetosphere and ionosphere by the propagation of shear mode Alfvï¿½n waves that propagate along the magnetic field and carry field-aligned current. The presence of Alfvï¿½n waves in the auroral zone can be observed from the ground by magnetometer arrays that detect the magnetic perturbations of these waves. The theory of the production of these ground signatures is well established for long period waves, but it is more complicated for the waves near one second period associated with the aurora. This group has developed a two-dimensional MHD code to describe this propagation. With this code, they have determined the effects of the atmosphere at modifying the Alfvï¿½n wave signature as observed on this ground. The first version of this code considered a system that was homogeneous in the horizontal direction, an assumption that fails in the auroral zone where density cavities confined in the horizontal direction are observed. The researchers have developed a model to include such horizontal inhomogeneities in a simplified version of the code, and this is being extended to the full code. In addition, they are extending the model to three dimensions to more realistically model the ground signatures of localized current distributions.

The final project involves the acceleration of electrons in Alfvï¿½n waves, and this model is extended to treat ions. The ion calculation is complicated by the fact that while the electrons can be treated in the guiding center approximation, the full ion dynamics must be included since the Alfvï¿½n waves can have perpendicular wavelengths that are small compared to the ion gyroradius. These test particle models can produce non-Maxwellian particle distribution in the electrons and ions. By combining these codes, the group is able to provide more complete predictions for the particle and wave measurements made along auroral field lines. These predictions are then compared with results from the recently launched Polar and Fast Auroral Snapshot (FAST) satellites.

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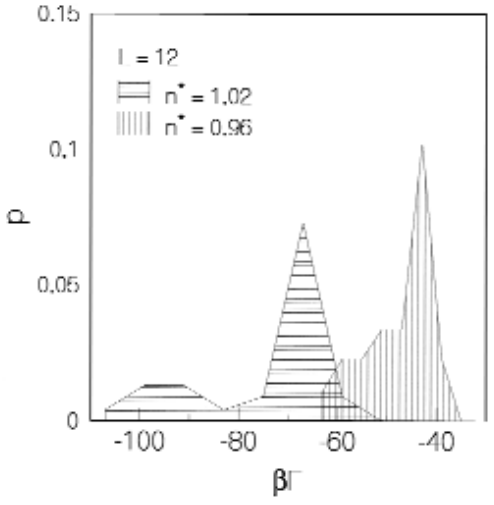
Numerical Studies in Condensed Matter Theory

This group is continuing their study of the properties of superconductors with unconventional pairing states. In one project, the researchers are using the numerical methods they have developed to solve the nonlinear London equations to compute the magnetic penetration depth as a function of the angle between crystallographic axes and applied magnetic field. In a second task, they are using numerical Renormalization Group methods to study finite size effects in the normal to superconductor phase transition in layered superconductors. A third task being undertaken is the calculation of the tunneling spectra in junctions between a ferromagnet and an unconventional superconductor. In a fourth task, the group is studying transport properties of layered superconductors along the crystallographic c-axis. In addition to high-temperature superconductors, this group is emphasizing other materials in which evidence for unconventional superconductivity has been accumulating. These include heavy fermion compounds, organic salt superconductors, and certain cubic perovskites to name a few.

Further work is being done on the microcanonical Monte Carlo method developed by this group. This method has made computational efficiency of simulations considerably better than that of conventional Monte Carlo procedures. This method is being used and extended to continue the study of the topography of the phase space (the structure of metastable minima separated by local maxima) of a glassy system. The current emphasis is on the inclusion of the effects of defects and impurities through the introduction of a random potential in the simulation. As a new task in this area, the group is beginning a study of freezing. They plan to develop their ideas in terms of general considerations applicable to the freezing transition in systems such as liquid crystals that exhibit a succession of phases.



Density of states for glassy free energy minima obtained from a novel Monte Carlo procedure to study

the free energy landscape of a glassy hard sphere system. Results at two densities are shown. (To appear in Physical Review E).

Research Group

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Igor Zutic, Research Associate
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Thomas F. Walsh, Fellow

Lattice Studies of the Gluon Propagator

These researchers are studying the gluon propagator on large lattices. The lattices from which the propagators are calculated can also be used to calculate hadron properties and are generated using full quantum chromodynamics (QCD) with Kogut-Susskind fermions. These researchers use the Hybrid Monte Carlo method that makes use of molecular dynamics techniques. Their techniques and numerical methods are of interest to many researchers seeking to optimize similarly complicated algorithms on MPP systems and on the Cray T3D supercomputer in particular.

Research Group

Henley Quadling, Graduate Student Researcher
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Theoretical Physics Institute

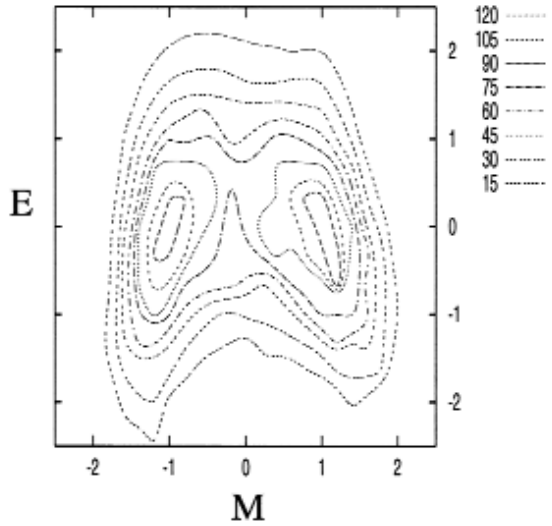
Philippe de Forcrand
Leonid Glazman
Larry McLerran

Philippe de Forcrand, Fellow

The Deconfinement Phase Transition in One-Flavor Quantum Chromodynamics

These researchers studied the deconfinement phase transition of one-flavor Quantum Chromodynamics (QCD) using the multiboson algorithm. The mass of the Wilson fermions relevant for this study is moderately large, and the non-hermitian multiboson method is a superior simulation algorithm. Finite size scaling is studied on lattices of size 83 X 4, 123 X 4, and 163 X 4. The behaviors of the peak of the Polyakov loop susceptibility, the deconfinement ratio, and the distribution of the norm of the Polyakov

loop are all characteristic of a first-order phase transition for heavy quarks. As the quark mass decreases, the first-order transition gets weaker and turns into a crossover. To investigate finite size scaling on larger spatial lattices, these researchers use an effective action in the same universality class as QCD. This effective action is constructed by replacing the fermionic determinant with the Polyakov loop identified as the most relevant Z(3) symmetry breaking term. Higher-order effects are incorporated in an effective Z(3)-breaking field, h, which couples to the Polyakov loop. Finite size scaling determines the value of h where the first order transition ends. This analysis, at the endpoint hep, indicates that the effective model and QCD are consistent with the universality class of the three-dimensional Ising model. Matching the field strength at the end point hep to the k values used in the dynamical quark simulations, the group estimated the endpoint hep of the first-order phase transition. They found hep ~ 0.08, which corresponds to a quark mass of about 1.4 GeV.



Distribution of the magnetization M and energy E at the second-order endpoint of the deconfinement transition line.

Research Group

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Leonid Glazman, Principal Investigator

Monte-Carlo study of Vortex Phase Diagram in Layered Superconductors

Thermodynamics and transport properties of Type II superconductors in magnetic field are essentially properties of the "vortex matter." A peculiarity of high Tc superconductors is a very high amplitude of thermal fluctuations in the vortex state. This leads to destruction of the low-temperature vortex crystal

state well below the mean field upper critical field. The only way to obtain quantitative information about the phase diagram in the vortex state is large-scale numerical simulations.

The researchers at the Theoretical Physics Institute have used time provided by the Supercomputing Institute to study the phase diagram by Monte-Carlo simulations of the three-dimensional, uniformly frustrated XY model. They have investigated the properties of the melting transition for different anisotropy parameters. The study shows that the pancake alignment above the melting transition increases with decreasing of the anisotropy. At high anisotropies, the melting is accompanied by a significant drop in the coupling energy and the destruction of vortex lines, while at small anisotropies the vortex lines preserve their continuity at the melting transition. In the linelike melting regime, the researchers find several universal properties of the transition and of the liquid phase. These properties include the scaling of the melting temperature with anisotropy and magnetic field, the effective line tension of vortices in the liquid regime, the latent heat, the entropy jump per entanglement length, and relative jump of Josephson energy at the transition as compared to the latent heat. Simulations advanced understanding of the vortex phase diagram in layered high-temperature superconductors.
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Larry McLerran, Principal Investigator

Improved Actions for Quantum Chromodynamics on Anisotropic Lattices

To achieve accurate results from lattice Quantum Chromodynamics (QCD), it is necessary to improve the lattice actions used in simulations. In the Symanzik improvement program, which this group is pursuing, one adds higher dimensional operators to the action (and currents) to eliminate the leading discretization errors affecting rotational or chiral symmetry. The so-called Schrodinger functional has recently become a powerful tool in eliminating the O(a) errors (a = lattice spacing) violating chiral symmetry non-perturbatively in the coupling. This tool is helping to eliminate the O(a) errors of quark actions on anisotropic lattices. This finally allows accurate simulations of heavy quarks.

As a first step in carrying out the program of QCD on anisotropic lattices (with spatial spacing a_s and temporal spacing a_t) with improved actions, the Schrodinger functional method was used to determine the renormalization of the anisotropy (a_s / a_t). This involves Monte Carlo measurements at various anisotropies as well as various gauge couplings (related to the lattice spacings).

Previous work has generated approximately 350 configurations at bare anisotropy 2 and only 20 configurations for thermalization of the system at anisotropy 4. This has been done for only one value of the coupling (beta) corresponding to a moderately coarse lattice. In order to achieve accurate statistics, at least 500 configurations are needed for each anisotropy at each coupling. These configurations are used for purposes beyond understanding the renormalized anisotropy. The same configurations are used in the improvement of the quark action on anisotropic lattices, which leads to accurate simulation of heavy quark systems.
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Medical School

Department of Cell Biology and Neuroanatomy

Edward Egelman
Christopher N. Honda
Steven Mcloon
Ernest Retzel
Martin W. Wessendorf

Edward Egelman, Principal Investigator

Understanding Molecular Motions in Protein Polymers by Three-Dimensional Reconstructions

Electron microscopy of negatively stained or unstained frozen-hydrated specimens provides information needed to produce three-dimensional reconstructions of macromolecular complexes. For many systems, electron microscopy is the only technique capable of visualizing active complexes of proteins and nucleic acids. This laboratory has been concentrating on two biologically important protein polymersï¿½actin and RecA. Actin is perhaps the most abundant and conserved eukaryotic protein, and it is involved in muscle, cell motility, and the control of cell shape and form. Since the E. coli RecA protein is capable (in vitro) of catalyzing the most important steps of homologous recombination between two DNA molecules, it has become the most intensively studied enzyme of general recombination. The steps that occur in this laboratory after images are acquired with an electron microscope are highly computational. Fourier-Bessel analysis and inversion are used to recover three-dimensional information from two-dimensional images of helical polymers, and work is in progress on both actin and RecA to understand the conformational dynamics of these polymers that result from nucleotide hydrolysis and interactions with different ligands. Furthermore, atomic resolution crystal structures of both actin and RecA are now available. Using electron microscopy and image analysis, these researchers have been able to understand some changes that must occur between crystal structures and active polymeric forms of both RecA and actin. This work is currently generating a wealth of structural information that is advancing the understanding of the function of these molecular assemblies.

Research Group

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Christopher N. Honda, Principal Investigator

Three-Dimensional Analysis of Spinal Cord Tissue

The goals of this project are to determine spatial relationships between opioid-receptor containing axon terminals of sensory neurons and projection neurons in the spinal cord. Data consists of stacks of

images of dual-colored immunofluorescence material collected using a confocal laser scanning microscope. Each stack of images contains a single neuron stained with one fluorophore and axon terminals marked with another.

Before being analyzed further, each stack of images must be processed using deconvolution software (Huygens) residing on certain workstations in the Basic Sciences Computing Laboratory. The group is using this laboratory because the deconvolution process is critical to their research and because similar computing power is beyond the reach of their laboratory.

Research Group

Anie Roche, Research Associate
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Steven Mcloon, Principal Investigator

Eph Receptor Tyrosine Kinases and Development of the Pattern of Connections in the Visual System

Axons of retinal ganglion cells connect to cells in the visual centers of the brain in a precise, stereotypical pattern. This pattern of connections is essential for normal visual function. The goal of this project is to further understanding of how the proper pattern of connections develops between retinal axons and the central visual centers. This project is guided by the hypothesis that the pattern of retinal connections in the brain is establishedï¿½in partï¿½due to interactions between sets of cytochemical positional labels carried by the retinal axons and by the cells in the target centers to which the axons connect. This project is a continuing effort by this laboratory to identify these positional labels. Available evidence suggests that gradients of specific Eph receptor tyrosine kinases expressed across the retina could be involved in detecting positional labels in the central visual centers. The role of these receptors in development of the visual system has never been directly tested. The overall aim of this project is to determine the role of members of the Eph subfamily of receptor tyrosine kinases in development of the normal pattern of retinotectal connections. In general, the approach to this project is altering the expression by retinal cells of specific receptors and then studying the resulting pattern of retinotectal connections in developing chick embryos.

Research Group

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Dan Selski, Research Associate
Amila Silva, Graduate Student Researcher
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Ernest Retzel, Principal Investigator

Comparative Genomics of Multiple Plant Species

These researchers are currently conducting a comprehensive comparative study of several plant

genomes. This study involves gathering genomic sequence and map data and combining it together in a single data source. In addition, this group is executing similarity search programs on every sequence to determine the similarities of each sequence to known proteins and to other sequences within each of the plant genomes. This similarity data and additional data from gene expression experiments is used as input to novel data mining techniques for determining clusters of genes within genomes and for comparing these clusters across genomes. Along with the data from genetic mapping experiments, this information provides a more comprehensive view of the genomes of plant species than is currently available. The similarity information is generated using similarity search programs such as BLAST and FASTA.

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Martin W. Wessendorf, Principal Investigator

Digital Restoration of Biological Images

Microscopic imagesï¿½even those from a confocal microscopeï¿½inevitably contain information that is out of focus. This out of focus information introduces blurring and decreases the resolution of which the microscope is capable. However, if one knows the point-spread function of the microscope, it is possible to back-calculate the object that would produce a given blurred digital image. This group is using a commercially available (but hardware intensive) software package (NUYGENS2, from Scientific Volume Imaging) to obtain biological images of greater resolution than currently possible. Subsequently, the researchers will use such restored images with a synaptological reconstruction program (DFIELD) currently under development to identify potential synapses in images of nerve cells.

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Department of Laboratory Medicine and Pathology

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William B. Gleason
Franz Halberg
Stephen S. Hecht

Lynda B.M. Ellis, Principal Investigator

Biocatalysis/Biodegradation Databse

Supercomputing facilities are being used by this researcher to support activities of the University of Minnesota Biocatalysis/Biodegra-dation Databse (UM-BBD). The UM-BBD is a database of microbial biocatalytic reactions and chemical compounds. The goal of the UM-BBD is to provide information on microbial enzymecatalyed reactions that are important for biotechnology. The reactions covered are studied for basic understanding of nature, biocatalysis leading to specialty chemical manufacture, and biodegradation of environmental pollutants. Individual reactions and metabolic pathways are presented with information on the starting and intermediate chemical compounds, the organisms that transform the compounds, the enzymes, and the genes. The present database has been successfully used to teach enzymology and use of biochemical Internet information resources to advanced undergraduate and graduate students, and is being expanded primarily with the help of such studens.
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William B. Gleason, Fellow

Theoretical and Experimental Studies of Systems of Biomedical Importance

Fibroblast Growth Factor (FGF), Vascular Endothelial Growth Factor (VEGF), and Bone Morphogenetic Protein (BMP) are all heparin-binding proteins. This group has been interested in the mechanism of recognition of glycosaminoglycans (of which class of compounds heparin is a member) for some time. FGF is important in wound healing, VEGF in the formation of new blood vessels, and BMP in the ectopic development of bone. All of these proteins have great potential for use as therapeutic agents. Tissue Interstitial Nephritis antigen (TIN-ag) is a protein of unknown biological function that is important in a type of kidney disease. The Fab/Cytc (complexes of the mouse self-antigen cytochrome c with monoclonal antibodies) system is of interest both for insight that may be gained into the process of antibody maturation in response to a protein antigen and as an example of a system for learning about autoimmunity.

This group has previously simulated the binding of heparin to FGF and is extending this work by initiating studies with VEGF and BMP in order to learn about their interactions with heparin. The main goal is to select a suitable molecular dynamics system, from ones available, for long-term use in studying the systems.

This group is also working with stents. Stents are currently used in a large percentage of cases involving balloon angioplasty. After an arterial obstruction is removed, the damaged blood vessel frequently becomes obstructed again (retenosis) due to an over enthusiastic biological response to injury. Metal stents have been deployed in a (partially) successful attempt to prevent retenosis.

This group is currently modifying the existing stent/rigid wall arterial model to include fluid elements to evaluate the anticipated high shear, turbulence, and recirculation effects of incomplete stent deployment in the fully expanded and partially occluded arterial lumen.

Research Group

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Franz Halberg, Principal Investigator

Chronobiologic Assessment of Physiologic Chronomes from Womb to Tomb

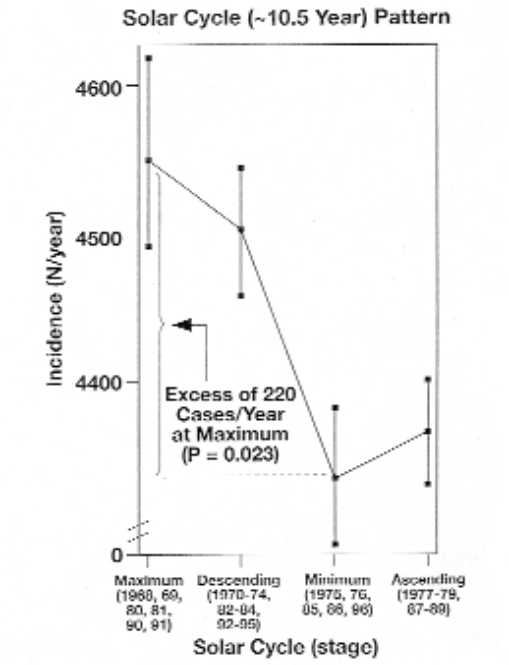
Strokes and other adverse vascular events are major cripplers at an estimated yearly cost of over $30 billion. A system for the chronobiologic analysis of cardiovascular records is being developed with a focus on disease prevention. Ambulatory devices are now used in different geographic locations for automatic monitoring of blood pressure and an electrocardiogram for seven days at the outset. Chronobiologic analyses of such records serve first and foremost to improve screening, diagnosis, and treatment. They also serve, from a basic viewpoint, to assess how environmental factors affect human physiologyï¿½notably heart rate and blood pressure. This group's pursuit of these goals is greatly facilitated by supercomputer access to analyze beat-to-beat records for resolving chronobiologic and chaotic endpoints, to automatically update reference standards as added data accumulate, to detect the earliest risk by means of chronome alterations, and to follow-up at-risk individuals longitudinally by means of control charts.

Toward this goal, several new programs are being developed, and these and existing programs are routinely applied for analysis of data as it accumulates. Existing records are to be organized into databases so that reference values can be regularly updated, and any abnormality can be easily detected. A library of programs for such chronobiologic applications is being organized and integrated with the incorporation of graphic displays for results.

A reduced heart rate variability is associated with a 550% increase in the risk of coronary artery disease, whereas an excessive circadian blood pressure amplitude (CHAT, or circadian hyperamplitude-tension) is associated with a 720% increase in the risk of cerebral ischemic events. Differences in the

correlation dimension of patients with coronary artery disease are observed by nightï¿½but not by dayï¿½rendering a chronobiological approach mandatory. About-weekly and other low-frequency components become more pronounced with advancing age and may provide added information on cardiovascular disease riskï¿½notably since they are now found to be amplified after coronary artery bypass grafting.

Environmental effects on heart rate variability and on other aspects of human physiology are slowly being recognized. In particular, exposure to magnetic storms is associated with a decrease in heart rate variabilityï¿½apparently in spectral regions away from ~1/3.6 seconds (suggesting mechanisms other than the parasympathetic). In turn, a decrease in heart rate variability may be a mechanism underlying the increase in myocardial infarctions in relation to stormy weather in space. In Minnesota, there is an excess of 220 deaths per year from myocardial infarction during years of high versus low solar activity. Cross-spectral techniques relating the biological information to physical records (also available at short intervals for very long spans, some covering several hundred years) thus gain in interest from a basic viewpoint as well.



Non-random patterns (means ± SEs) of incidences of mortality from myocardial infarction in Minnesota (1968ï¿½1996). These include, with about-weekly (peak on Mondays) and about-yearly (peak in the winter) changes (not shown), variations as a function of the about 10.5-year sunspot activity cycle. In comparison with times of solar minimum, times of solar maximum show an excess of 220 deaths per year due to myocardial infarction.

Research Group

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Stephen S. Hecht, Principal Investigator

Biochemistry, Biology, and Carcinogenicity of Tobacco-Specific N-Nitrosamines

The evidence that tobacco-specific nitrosamines (TSN) play an important role in cancer induction by tobacco products is strong. Smoking is by far the major cause of lung cancer, a disease that is expected to kill 1.16 million people. NNK, 4-(methylnitrosamino)-1-(3-pyridyl)-1-butanone, and polycyclic aromatic hydrocarbons (PAH) are the most prevalent pulmonary carcinogens in tobacco smoke. Smoking is an important cause of esophageal and pancreatic cancer, being responsible for 70ï¿½80% of esophageal cancer death and 25% of pancreatic cancer death in the United States. N'-nitrosonornicotine (NNN) occurs in greater concentrations in cigarette smoke than any other esophageal carcinogen. NNK and its major metabolite NNAL, 4-(methylnitrosamino)-1-(3-pyridyl)-1-butanol, are the only known pancreatic carcinogens in cigarette smoke. While the complexity of tobacco smoke precludes definite assignment of cause and effect to any particular carcinogen, NNK, NNAL, and NNN certainly play a significant role in cancer induction. The overall goals of this project are to determine carcinogen metabolic activation and detoxification pathways, to elucidate the structures of the DNA adducts that are formed in the activation process to determine the significance of these adducts in carcinogenesis, to understand structure-carcinogenicity relationships, and to develop methods that can be used to detect relevant metabolites, protein adducts, or DNA adducts in humans.

Research Group

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Department of Microbiology

Ronald Jemmerson, Principal Investigator

Three-Dimensional Animation and Multimedia for Scientific Visualization

Using the resources of the Basic Sciences Computing Laboratory, this group is pursuing their interests in immunoglobulin specificity to the front of multimedia. They are using three methods of data collection for these projects. The first involves accessing the Brookhaven database for known biochemical structures to use for pibt data in setting up three-dimensional animation using various Molecular Modeling programs and porting the structures in Silicon Graphics Inc., Blender. The second method of data collection is X-ray crystallography of immunoglobulin fragment antigen-binding-cytochrome c complexes for modeling. The final method is confocal laser-scanning microscopy for volume rendering. The three-dimensional animations are then ported to Windows NT at the University of Minnesota Cell Biology and Neuroanatomy's Biomedical Image Processing Laboratory for multimedia and sprite animations using Director and Animator Studio for video and RealVideo and

MPEG publishing on the Computational Biology Center's Solaris World Wide Web servers.

Research Group

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Department of Orthopaedic Surgery

Jack L. Lewis, Principal Investigator

Biomechanics of Articular Cartilage

This work requires the use of ABAQUS to study the stresses that arise in various joint tissues. This work is part of an interdisciplinary research program intended to understand the cause of osteoarthritis, a degenerative joint disease, utilizing both biomechanical and biological/biochemical methodology. The calculated stresses from ABAQUS are correlated to experimentally observed histological damage and failure criteria for the joint tissues. The modeling of the biological tissues require the use of large strain formulations and nonlinear constitutive relationships as well as nonlinear contact parameters.

Previous work resulted in the development of a finite element mesh of the joint, and several tests were run to verify the mesh density and contact conditions. A hyperelastic constitutive model for the cartilage layer in the model was fitted to experimental stress-strain measurements using ABAQUS and IMSL routines. Two experiments were analyzed using the model. Damage following acute impactions and damage two weeks following impaction were looked at. The results from the two studies have suggested that cracks in the cartilage surface layer result from forces other than the vertical force generated directly by the impaction. The finite element analyses also indicated a tensile strength for subchondral bone of approximately 70 MPa. The calculated stress distributions did not correlate with the observed pattern of cell death in the tissue indicating that deep cells in the tissue may be less susceptible to damage than their counterparts near the surface.

Research Group

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Return to Top

Department of Pharmacology

Duanqing Pei
George L. Wilcox

Duanqing Pei, Principal Investigator

Matrix Metalloproteinases and Their Inhibitors

A family of enzymes called matrix metalloproteinases have been implicated in a number of disease states ranging from arthritis to tumor invasion and metastasis. The structure-function of matrix metalloproteinases is a main area of research in this group within the broader context of their roles in tumor invasion and metastasis. These researchers believe that the unique function associated with each enzyme can be best understood with the knowledge of three-dimensional structures. To this end, these researchers are expressing three members of this gene family and are crystallizing them for X-ray diffraction and three-dimensional structure determination. Aided with the structural data, they are synthesizing inhibitory compounds for these enzymes that can be used in research as well as in the development of new drugs for arthritis and cancer.

Research Group

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George L. Wilcox, Fellow

Spatial Propagation of Impulses in Excitable Cells

This project is a long-term multidisciplinary endeavor involving the fields of molecular and cellular biology, computer science, pharmacology, and mathematics. Biophysically detailed models of impulse propagation in excitable cells have been studied with mathematical models since 1952. The equations used were a system of four partly dissipative semilinear parabolic differential equations, typically with Neumann boundary conditions. Over the years, more complexity has been added to the basic model, and typical systems today may comprise systems of twenty to thirty coupled nonlinear differential equations. Such equations have been an area of intense study by biologists, mathematicians, and computational scientists. Due to the nonlinear nature of the equations, there is very little hope of obtaining analytical solutions. The only option available is to compute numerical solutions.

In the recent past, the widespread use of techniques of molecular biology has made it possible to sequence and clone the mechanisms responsible for cellular excitability such as cell membrane ion channels and ion pumps. In addition, by expressing genes responsible for ion channels in cells, it has become possible to study the detailed kinetics of these channels and dissect the components of cellular excitability at a molecular level. In addition, the result of mutations can also be studied allowing the investigation of serious genetic defects. Finally, it is possible to construct mathematical models of the action of various drugs at the molecular, cellular, and tissue levels.

This group is simulating the electrical activity of three types of cells. Collaborators in the University of Leicester have constructed carrier DNA (cDNA) libraries for such cells and have started constructing databases of ion channels with information about kinetics and pharmacology. With this molecular information, this group is in a position to construct models for propagation of electrical activity in single nerve fibers and networks of sinoatrial node cells. In addition to numerous questions about the normal physiology of these systems, the effects of mutations and drugs can be effectively studied.

Other work applied evolutionary algorithms (EAs) to the problem of parameter selection in the high-dimensional spaces describing finite element (compartmental) models of neurons. In this work, the researchers explored the scalability of parameter spaces and searches by extending their results to large-scale models with biophysically realistic morphologies. The work is continuing the development of the CA3 hippocampal model and is currently beginning the exploration of a cerebellar Purkinje cell model. The researchers are interested in the importance of variability in the form and function of the nervous system, in particular the density of ion channels. The group is seeking to predict values critical to their understanding of neural function, but that are missing from the neuroscientific literature due to measurement limitations in experimental technologies. The suite of tools being developed to support this project enables neuroscientists, as well as researchers in other fields, to optimize parameter combinations and explore the significance of selected parameters in their simulated systems.

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Department of Physiology

David Levitt
Robert F. Miller

David Levitt, Principal Investigator

Determination of Protein Structure from X-ray Diffraction Data

These researchers are refining the X-ray crystallographic structure of the human liver bifunctional enzyme. This protein plays a central role in the control of blood glucoseï¿½reciprocally regulating both glycolysis and gluconeogenesis. The activity is regulated through the phosphorylation of the protein. This is a collaborative project with another laboratory that has developed two mutant forms of the enzyme to mimic either the phospho or dephopho state of the enzyme. The group is working to determine the structure of both forms. These structures help elucidate the mechanism by which phosphorylation alters the kinetic properties of the enzyme. If successful with these two enzymes, there are a number of mutations planned for study.

There have been huge technical advances in recent years in the solution of protein structures by X-ray crystallography. The combination of Synchrotron X-ray sources and Selenomethionine Multi-wavelength Anomalous Dispersion (SMAD) phasing techniques has made the generation of high-resolution electron density maps a routine procedure. The most time consuming step now is the building of the initial protein structure into the electron density map. Currently, this requires several weeks of a skilled investigators time working at a high-performance graphics station. These researchers have begun developing a program to automate this procedure. The goal is to be able to submit the electron density map and the amino acid sequence to the computer, which returns an accurate initial structure that can be used as input to refinement programs. Considerable progress has already been made in the development. Presently, this group is able to automatically fit nearly all the secondary structure. The next step is to extend these secondary structures into the loop regions. It is then possible to assign the amino acid residues, complete the loops, and refine the side chain atom positions. The development of this program requires extensive time on a graphics workstation. Each step in the fitting process is monitored using a protein visualization program that has been developed specifically for this project.

Research Group

Timothy A. Anderson, Research Associate
Ethan P. Bernard, Supercomputing Institute Undergraduate Intern
Seth T. Gammon, Supercomputing Institute Undergraduate Intern
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Robert F. Miller, Principal Investigator
Jon Gottesman, Co-Principal Investigator

Computational Modeling of Synaptic Transmission and Electrophysiology of Cells in the Retina

This project is enhancing the understanding of amacrine and ganglion cell function in the vertebrate retina through a tightly coupled project of computer simulation analysis combined with physiological and morphological studies of single cells. There are three broad objectives in this project.
The first objective is a new understanding of how ganglion and amacrine cells in the vertibrate retina generate nerve impulses and the role which voltage-gated ion channels in the dendrites play in impulse encoding. The next objective studies the mechanisms of glutamate release from ribbon synapses of bipolar cells and the role of diffusion and glutamate uptake in shaping the temporal waveform of the glutamate concentration profile in the synaptic cleft that interacts with different glutamate receptors and glutamate transporters. The final objective is studying the role that the different glutamate receptors play in the generation of synaptic currents integrated by active or passive soma-dendritic tree structures. Computer simulations are being carried out for equivalent cylinder and compartmental models of cells using the NEURON software package. Modeling of synaptic transmission and glutamate release, diffusion, and uptake are being done using MCELL simulator software.

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Department of Psychiatry

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Functional Brain Imaging of Pain

This project uses functional magnetic resonance imaging to evaluate chronic pain in a rat. Chronic pain models are simulated using a persistent inflammation model and a nerve injury model. This research helps in understanding the etiologies of chronic pain and is developing models for targeting pharmacologic therapies.

Research Group

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Department of Radiology

Patrick W. Mantyh, Principal Investigator

Functional Brain Imaging of Pain

This project deals with three-dimensional reconstruction of medical imagesï¿½digital subtraction angiograms from limited number of two-dimensional biplane angiograms with cone beam geometry. The voxel based reconstruction model uses an iterative technique and a new method for calculating the weighting function by computing the intersection volume between two convex bodies (a cubic voxel and a pyramidal X-ray beam). To date, these researchers have demonstrated reconstruction of three-dimensional volumes with 2563 voxels. Current work aims to demonstrate clinical applications that require a resolution of 5123ï¿½or moreï¿½voxels in a reasonable time.

Research Group

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Department of Surgery

Kristen Gillingham
Carl S. Smith

Kristen Gillingham, Principal Investigator

Random Assignment of Treatments in Solid Organ Transplant Research

In solid organ transplant research, many randomized clinical trials are conducted. These researchers have written a program in FORTRAN 77 that has allowed them to carry out the random assignment of various treatments to their study patients. This randomization program requires access to the IMSL library and is currently being run through Supercomputing Institute resources.

Research Group

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Department of Radiology

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Three-Dimensional Reconstruction of Cerebral Vasculature

This project deals with three-dimensional reconstruction of medical images - digital subtraction angiograms from limited number of two-dimensional biplace angiograms with cone beam geometry. The voxel based reconstruction model uses an iterative technique and a new method for calculating the weighting function by computing the intersection volume between two convex bodies (a cubic voxel and a pyramidal X-ray beam). To date, these researchers have demonstrated reconstruction of three-dimensional volumes with 2563 voxels. Current work aims to demonstrate clinical applications that require a resolution of 5123-or more-voxels in a reasonable time.
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Carl S. Smith, Principal Investigator

Dynamics of Urethral Sphincter Activity

Dynamical analysis is a mathematical tool that provides a powerful alternative to traditional biologic signal processing. Traditional approaches quantitate and characterize signals by parameters such as frequency, amplitude, and waveform in an effort to discover the underlying relationships within the system under study. A dynamical approach utilizes the same time dependent information but constructs a visual picture, an attractor, of the nature of interaction found with the system that generated the signal. This is an extraordinary unexpected result in dynamical analysisï¿½that isï¿½for the first time, a technique that allows a glimpse at the richness of structures that create the biologic signal. Furthermore, despite the apparent system complexity, a dynamical analysis can reveal a series of simple rules that govern the systems behavior. This study examines the electromyographic (EMG) signal present in the urethral straited muscle during bladder filling.

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Dynamic Simulations of Solvated Protein-DNA Complexes

The Estrogen Receptor (ER) and glucocorticoid receptor (GR) are DNA regulatory proteins. Several genes associated with cancer are regulated by these proteins, and considerable work has been published on their characterization. In addition, DNA sites to which the ER and GR bind specifically and induce

gene transcription have been well characterized. However, the underlying mechanism as to how the receptors recognize and bind to DNA have not been defined. An understanding of this DNA recognition event has many potentially beneficial applications for controlling tumor growth and expression.

These researchers are computing molecular dynamics simulations of an ER DNA Binding Domain/estrogen response element (ER DBD/ERE) complex in a 10 Angstrom water layer. The simulations and polyacrylamide gel shift findings have suggested the ER and GR proteins may function in a similar manner as a genetic switch at non-consensus Glucocorticoid Response Element (GRE) and ERE DNA sites. Investigations of this hypothesis are being conducted in wetwork experiments.

It was recently observed, using a gel shift assay, that the GR protein specifically binds to a non-consensus ERE and to a nucleotide sequence within the coding region of the ER gene that encodes the ER DNA recognition helix. This finding has far reaching implications and may explain the differential regulation of steroid hormone receptor gene expression. The finding also points to the design of genetically engineered expression vectors to selectively block gene expression among the steroid hormone receptor protein family.

Recently, in wetwork experiments, this group was successful in obtaining carrier-DNA clones of Mouse Mammary Tumor Virus (MMTV) proviral DNA from mouse mammary tumor tissue. These clones contain hormone response elements that bind the GR protein. In addition, two of the clones contain a cellular oncogene on their ends. The GREs found in these MMTV proviral carrier-DNA clones were found to differ in nucleotide sequence from the consensus GRE in the long terminal repeat upstream from the MMTV gene transcription initiation site.

Current findings with the ER and GR proteins are similar to those described for the 434 bacteriophage cI and cro repressor proteins interacting at adjacent operator sites. The proteins interact at the same operator sites and differentially induce gene expression functioning biologically as a classical genetic switch. The cro binds in order of preference for operator sites OR3 > OR2 > OR1 and induces gene transcription upstream from the sites, and the cI binds for operator sites OR1 > OR2 > OR3 and induces transcription downstream from the sites.

Further work is continuing with genetic engineering experiments designed to turn on or off gene transcription under the regulation of the ER and GR proteins. Interactive work is being done with both benchwork and computational methodology using the information gained to design laboratory experiments and to refine the computer models. Finally, molecular dynamics simulations on 434 cI repressor protein in complex with operator sites is being conducted (see figure 1). Models have also been constructed in a 10 Angstrom water layer of the 434 cro protein in complex with operator sites (see figure 2). Computations of these models are underway.

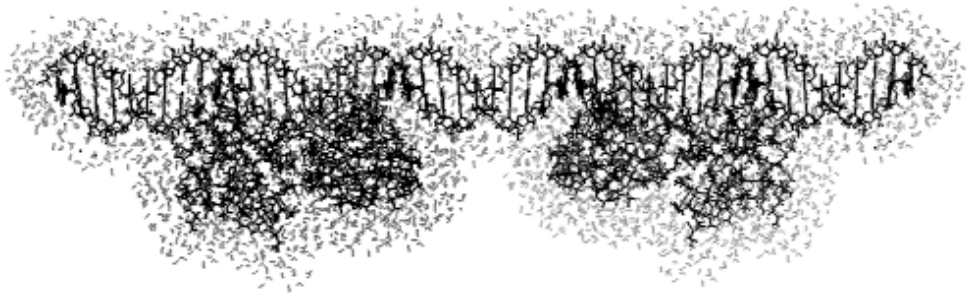

Figure 1: Two 434 cI protein dimers in complex with a 51bp DNA sequence containing operator sites OR1 and OR2. The protein dimers are docked at their cognate binding sites on the DNA and the

complex is solvated with a 10 Angstrom water layer.

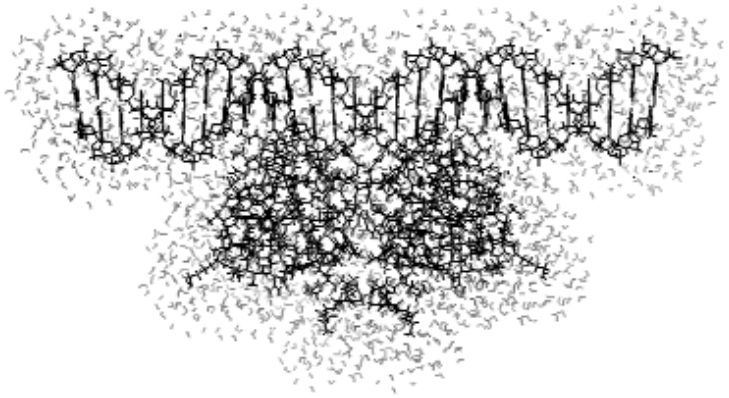

Figure 2: A 434 cro protein dimer in complex with a 28bp DNA sequence containing operator site OR3. The protein dimer is docked at its cognate binding site on the DNA and the complex is solvated with a 10 Angstrom water layer.

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University of Minnesota--Twin Cities Campus

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Department of Epidemiology

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Model-Intensive Genetic Analysis of Blood Pressure

High blood pressure is a major public health concern. More than twenty percent of the United States population will eventually be affected with high blood pressure (Hypertension). To date, no gene has been found that accounts for a significant proportion of the total inter-individual variation in blood

pressure. The difficulty in finding genes is due to the complex nature of blood pressure variation. It is believed that blood pressure is affected by multiple genes and multiple environmental factors.

Classical methods of finding genes for diseases assume that the disease is caused by a single gene. Cystic Fibrosis is an excellent example of a single-gene disease that has been located by single-gene methods. However, the classical methods, with their single-gene assumption, have been disappointing when applied to multi-factorial complex diseases. Statistical Genetics has developed two major approaches to this problem. The first and more widely used is abandoning explicit model-based methods and using non-parametric methods. The second is to increase the sophistication in the model (i.e., to use a two-gene model and introduce simultaneous correction for known environmental effects). A simulation study has been published that shows increased power for this approach, but the application of this approach has been hampered by the extreme computational demands of these models.

The availability of a massively parallel supercomputer makes it possible, for the first time, to use these two-gene models to analyze a real trait. The dataset available to this researcher is from the San Antonio Family Heart Study. This study is of approximately 1,200 individuals in 46 extended Mexican American families. The family structures have been recorded along with a huge database of relevant information including sex, age, health, diet, morphometrics, and 250 genetic markers scattered throughout the genome at an average spacing of approximately 15 centimorgans (the total genome length is approximately 3,300 centimorgans).

Maximum likelihood methods are used to construct the optimal model assuming two genes, two markers, and the covariatesï¿½sex, age, and body mass index. Other covariates are available and will be used if found to be significant. The maximum likelihood model under the assumption of linkage and no linkage are computed. The difference in these two likelihoods is considered a measure of the strength of linkage between the markers and the genes. This difference, called the lodscore, is considered significant when it exceeds the value 3.3.

This researcher is computing the lodscore for all 62,500 combinations of genes and markers for systolic blood pressure. Faster methods of performing the linkage that make different assumptions about the residual distribution are then explored. These other approaches should show a relatively small loss of power.

Research Group

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University of Minnesota--Twin Cities Campus

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Mitchell Abrahamsen, Principal Investigator

Molecular Characterization of the Cryptosporidium parvum Genome

Cryptosporidium parvum belongs to one of several protozoan genera that are referred to as coccidia in the phylum apicomplexa. It is an obligated intracellular parasite that develop in the gastrointestinal tract of vertibrates through all of its life cycle. Cryptosporidium infection is now a well-recognized cause of diarrhea in immunologically health and immuno-compromised humans and animals throughout the world. At the present time, there is no effective therapy for treating or preventing infection with C. parvum. Moreover, effective methods for subspecific differentiation (strain typing) and epidemiological surveillance (strain tracking) of this organism are not available. This is primarily due to lack of understanding of the basic cellular and molecular biology of this pathogen in terms of virulence factors, genome structure, gene expression, and regulation. Technically, there are neither successful in vitro culture systems that provide large amounts of parasite materials nor effective techniques for purification of the intracellular stages. Therefore, molecular biology studies are limited to those development stages for which large numbers of purified cells are available (i.e., sporozoites).

A prerequisite to understanding the complete biology of an organism is the determination of its entire genome sequence. In order to provide a fundamental knowledge of unique aspects of Cryptosporidium biology and host-parasite interaction at all stages of parasite development, this group has initiated a systematic genomic sequencing approach. The specific aims of these projects are to systematically sequence and annotate the two smallest C. parvum chromosomes, determine the developmental expression of putative genes identified, and to identify polymorphic DNA markers in C. parvum isolates and evaluate DNA fingerprinting strategies for the rapid and unambiguous differentiation of isolates.

Research Group

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College of Veterinary Medicine

Department of Management

Rakesh Kawatra, Principal Investigator

A Lagrangian Based Heuristic for the Design of Multipoint Linkages in a Communication Link with Unreliable Links and Node Outage Costs

This researcher is working to solve the topological problem of a local access network where communication links are unreliable, and the terminal nodes have associated outage costs. The mathematical model of the problem is an integer programming problem solved using Lagrangian relaxation techniques. Previous tests on smaller problems indicate that this solution method yields good results, and current work is focusing on testing the method on larger problems.

The program is written in FORTRAN, and the bulk of the computation in the program is in solving linear programming problems. Supercomputing resources are being used to solve these problems by making subroutine calls to the International Mathematical and Statistical Library (IMSL) routines that make efficient use of memory and processing time.

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Xiaoyang Zhu, Principal Investigator

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