2003 Annual Research Report of the Supercomputing Institute for Digital Simulation and Advanced Computation

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UNIVERSITY OF MINNESOTA

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for Digital Simulation and Advanced Computation
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Editor: Tracey Bartlett

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Table of Contents

Introduction

Supercomputing Institute Programs

Researchers and Administration

Conferences

Table of contents continued on next page

Ongoing and Recently Completed Research Projects from January 1, 2002 to March 15, 2003

Table of contents continued on next page

Table of Contents

Index and Bibliography

Index of Principal Investigators

Bibliography of Research Reports for January 1, 2001–March 15, 2003

Introduction

Overview

Founded in 1984, the Supercomputing Institute 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, high-performance network communications, informatics, and data mining.

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.

Digital Technology Center

The Supercomputing Institute plays a central role in the University of Minnesota's digital technology initiative. This initiative includes technologies based on computers, electronics, telecommunications, digital design, computational biology, systems recognition and verification, graphics and visualization, databases and data mining, networks, storage, artificial intelligence, robotics and vision, signal processing and wireless technology, and electronic commerce. Key to this initiative is the renovation of Walter Library on the University's East Bank Campus into a Digital Technology Center. This $63.4 million renovation kept the library's historic 1920s decor intact while revamping the interior to include state-of-the-art technology. The Supercomputing Institute joined the Digital Technology Center in 2001 and moved to the home of the Digital Technology Center in Walter Library in March 2002, where it is located on the fifth floor and part of the fourth floor and basement.

Supercomputers

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. From its inception through 1999, the supercomputing resources offered to the University of Minnesota research community have included a Cray-2, an ETA 10, a Cray X-MP, an IBM 3090, a Cray M90, a Cray T3D, a Cray C90, a Cray T3E-900, an IBM SP based on Silvernodes, and an IBM SP based on WinterHawk and NightHawk nodes.

The Supercomputing Institute has continued the strong tradition of providing University of Minnesota researchers with leading-edge, high-performance computing technologies and diversified programs that complement these technologies. In addition, the Institute has developed a strong program of user support, including tutorials and applications support across the physical, biological, mathematical, and computer sciences, engineering, and other disciplines that use high-performance computing, informatics, and data mining.

In April 2000, the WinterHawk nodes were upgraded to WinterHawk+ technology. The Institute's IBM SP supercomputer currently consists of a 370-processor supercomputer with 663 GB of memory. The nodes available for computation are:

- 74 4-processor WinterHawk+ nodes with 375 MHz Power3 processors; 16 nodes have 8 GB of memory each; the remaining nodes each have 4 GB of memory.
- 12 4-processor NightHawk nodes, each with 222 MHz Power3 processors and 16 GB of memory.

Four of the WinterHawk+ nodes are available for interactive use, and the remaining WinterHawk+ nodes and all NightHawk nodes are for computation through the queuing system. There are also four WinterHawk+ nodes used as file servers.

In addition, the Institute has a 16-processor Silvernode IBM SP with 12 GB of memory. The Silvernode SP utilizes the 332 MHz PowerPC 604e processor and has 4 TB of disk space. The IBM supercomputer resources are available in coordination with the IBM Shared University Research (SUR) partnership.

In March 2002, the Supercomputing Institute purchased an IBM pSeries 690 (Regatta). This system was upgraded in August 2002 to two Regattas. The system consists of two compute nodes with 1.3 GHz Power4 processors, file servers, and an interactive node. One of the compute nodes has 32 processors sharing 64 GB of memory, while the second node has 24 processors sharing 24 GB of memory. The interactive node is a WinterHawk+ node. Four 4-processor NightHawk nodes are used as file servers for 7 TB of disk.

The Institute's LINUX Cluster consists of 82 2-processor Netfinity nodes from IBM. Of these 82 nodes, 76 are available for computation, five are file servers, and one node is for interactive use. Seventeen of these nodes have two 733 MHx Intel Pentium III processors sharing 1 GB of memory. The remaining nodes have two 1.26 GHz Pentium III processors sharing 3.25 GB of memory. The nodes are connected together using Fast Ethernet and Myrinet. A cluster file system provides 2.5 TB of disk that can be used on all nodes.

The IBM systems will be upgraded in July 2003 and further upgraded in Fall 2003.

In May 2001, the Supercomputing Institute installed two 96-processor SGI Origin 3800s. Each SGI Origin 3800 has 144 GB of memory. These supercomputers utilize 500 MHz R14000 processors. The Institute also offers access to a 12-processor SGI Origin 2000 with 22 GB of memory. This Origin system will be replaced in June 2003 by a new SGI Altix system.

Continued on next page

Supercomputers (continued)

In 2003, the Institute installed a 32-processor Intel Xeon 2.0 GHz ES7000 Orion 230 supercomputer with 64 GB of memory, Windows 2000 Datacenter operating system software, and a 32-processor Microsoft SQL Server license.

These supercomputers offer the Supercomputing Institute's researchers access to state-of-the-art, high-performance computing technology. The Supercomputing Institute joined the Digital Technology Center in 2001, and in 2002 the supercomputing resources moved to new facilities on the East Bank of the Minneapolis Campus. 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 Computational Genetics Laboratory, the Digital Technology Computational Biology Laboratory, the Scientific Development and Visualization Laboratory, the Medicinal Chemistry/Supercomputing Institute Visualization–Workstation Laboratory, the Laboratory for Large-Scale Data Analysis, the Laboratory for Computational Science and Engineering, and interdisciplinary Ph.D. programs in Scientific Computing and Computational Neuroscience.

The major supercomputing resource program and long-term planning at the Institute are guided by the Institute's Planning Committee.

Planning Committee

Donald G. Truhlar, Supercomputing Institute Director, Chemistry, Chemical Physics, and Scientific Computation, *chair*

Graham V. Candler, Aerospace Engineering and Mechanics and Scientific Computation

James R. Chelikowsky, Chemical Engineering and Materials Science and Scientific Computation

Jiali Gao, Chemistry and Scientific Computation

Yiannis Kaznessis, Chemical Engineering and Materials Science

Vipin Kumar, Computer Science and Engineering and Scientific Computation

David J. Lilja, Electrical and Computer Engineering and Scientific Computation

Alon V. McCormick, Chemical Engineering and Materials Science

Douglas H. Ohlendorf, Biochemistry, Molecular Biology, and Biophysics

Yousef Saad, Computer Science and Engineering and Scientific Computation

George L. Wilcox, Neuroscience and Scientific Computation

Research Laboratories

Basic Sciences Computing Laboratory

Since 1996, the Supercomputing Institute has provided high-performance workstations and visualization equipment to enhance the research capabilities of the University community through the Basic Sciences Computing Laboratory, located in the Basic Science and Biomedical Engineering Building on the East Bank of the University of Minnesota–Twin Cities. The Institute manages this laboratory jointly with the Structural Biology Program. The facility occupies approximately 1,700 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 a variety of SGI workstations and an IBM Intellistation. The Supercomputing Institute provides technical support and user support for these high-performance computing resources, and the laboratory is available to all University of Minnesota researchers.

This laboratory was overseen and guided during 2002–03 by the following committees:

Executive Committee

Douglas H. Ohlendorf, Biochemistry, Molecular Biology, and Biophysics

Donald G. Truhlar, Supercomputing Institute Director, Chemistry, Chemical Physics, and Scientific Computation

Steering Committee

Kevin H. Mayo, Biochemistry, Molecular Biology, and Biophysics, *chair*

David H. Live, Biochemistry, Molecular Biology, and Biophysics

Kylie J. Walters, Biochemistry, Molecular Biology, and Biophysics

Martin W. Wessendorf, Neuroscience

Carrie M. Wilmot, Biochemistry, Molecular Biology and Biophysics

Darrin M. York, Chemistry and Scientific Computation

Research Laboratories (continued)

Computational Genetics Laboratory

The Supercomputing Institute recently created the Computational Genetics Laboratory in conjunction with the Center for Microbial and Plant Genomics and the Biomedical Genomics Center. The laboratory is designed to meet the emerging computational needs of the computational biology community, especially in the areas of genomics, bioinformatics, and computational genetics. The laboratory will be in St. Paul, and will be located in the new Microbial and Plant Genomics Building. User support in this area is also provided in the Basic Sciences and Biomedical Engineering Building, in the Medicinal Chemistry/Supercomputing Institute Visualization–Workstation Laboratory, and at the Supercomputing Institute main offices in Walter.

This laboratory was overseen and guided during 2002–03 by the following committees:

Executive Committee

Ronald L. Phillips, Agronomy and Plant Genetics

Ashley T. Haase, Microbiology

Donald G. Truhlar, Supercomputing Institute Director, Chemistry, Chemical Physics, and Scientific Computation

Steering Committee

Vivek Kapur, Veterinary Pathobiology, *chair*

Judith G. Berman, Genetics, Cell Biology, and Development

George Karypis, Computer Science and Engineering and Scientific Computation

Yiannis Kaznessis, Chemical Engineering and Materials Science

Arkady Khodursky, Biochemistry, Molecular Biology, and Biophysics

Lawrence P. Wackett, Biochemistry, Molecular Biology, and Biophysics

Research Laboratories (continued)

Digital Technology Computational Biology Laboratory

The Digital Technology Computational Biology Laboratory provides computing resources to faculty members involved in computational biology. While computational biology faculty have full access to all Institute resources, this laboratory is dedicated to computational biology in a way that allows special and focused stimulation of interdisciplinary and interdepartmental digital technology collaboration among University of Minnesota faculty and their research groups. The goal of the laboratory is to encourage collaboration and high-performance computing research within the computational biology community at the University of Minnesota. The laboratory is equipped with an 8-processor Compaq ES40 with a processor speed of 500 MHz and 8 GB of memory.

This laboratory was overseen and guided during 2002–03 by the following committees:

Executive Committee

Hans G. Othmer, Mathematics and Scientific Computation, *chair*

Donald G. Truhlar, Supercomputing Institute Director, Chemistry, Chemical Physics, and Scientific Computation

Steering Committee

Hans G. Othmer, Mathematics and Scientific Computation, *chair*

Jiali Gao, Chemistry and Scientific Computation

Alexander Y. Grosberg, Physics and Astronomy and Scientific Computation

John S. Lowengrub, Mathematics and Scientific Computation

Scientific Development and Visualization Laboratory

The Supercomputing Institute's Scientific Development and Visualization Laboratory, which is located in the Supercomputing Institute's facilities on the fifth floor of Walter Library, provides front-end equipment, including SGI, Sun, and IBM UNIX workstations, Macintosh workstations, an Intellistation from IBM running Windows NT, a color scanner, a CD writer, and a Macintosh workstation for the creation and manipulation of videos. The Institute provides user support services for supercomputer-related research using these general-purpose systems.

For 2002–03, the Scientific Development and Visualization Laboratory was guided by a faculty steering committee made up of:

Alon V. McCormick, Chemical Engineering and Materials Science, *chair*

Jiali Gao, Chemistry and Scientific Computation

Satish C. Gupta, Soil, Water, and Climate

Daniel M. Kroll, Pharmacy

Gary W. Meyer, Computer Science and Engineering

Henryk K. Stolarski, Civil Engineering

Research Laboratories (continued)

Medicinal Chemistry/Supercomputing Institute Visualization–Workstation Laboratory

The Medicinal Chemistry/Supercomputing Institute Workstation–Visualization Laboratory is co-sponsored 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 medicinal chemistry applications and scientific visualization.

This laboratory was overseen and guided during 2002–03 by the following committees:

Executive Committee

Yusuf J. Abul-Hajj, Medicinal Chemistry

Donald G. Truhlar, Supercomputing Institute Director, Chemistry, Chemical Physics, and Scientific Computation

Steering Committee

Rodney L. Johnson, Medicinal Chemistry, *chair*

David J. W. Grant, Pharmaceutics

Carston R. Wagner, Medicinal Chemistry

Laboratory for Large-Scale Data Analysis

This laboratory promotes use of the Unisys Orion computer for large problems and large data sets that demonstrate the capabilities of the hardware, operating system, and software.

For 2002–03, the Laboratory for Large-Scale Data Analysis was guided by a faculty steering committee made up of:

Yiannis Kaznessis, Chemical Engineering and Materials Science, *chair*

Fred Dulles, Coordinator of Information Technology, College of Biological Sciences

Jialo Gao, Chemistry and Scientific Computation

Vipin Kumar, Computer Science and Engineering and Scientific Computation

David J. Lilja, Electrical and Computer Engineering and Scientific Computation

Michael J. Olesen, Digital Technology Center, *ex officio*

Yousef Saad, Computer Science and Engineering and Scientific Computation

Graduate Programs

Scientific Computation Graduate Program

The graduate degree program in scientific computation encompasses coursework 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. The current Director of Graduate Studies is Jiali Gao of the Department of Chemistry.

Computational Neuroscience Program

The Computational Neuroscience Program is a unique interdisciplinary study and research program that combines neuroscience and computation. The program requires the use of quantitative methods and computer-related analysis techniques to study the development, structure, and function of the nervous system. The Supercomputing Institute is united with graduate programs in Biochemistry, Molecular Biology and Biophysics, Biomedical Engineering, Chemical Engineering, Chemistry, Chemical Physics, Computer Science, Mathematics, Neuroscience, Physics, and Scientific Computation to provide a new paradigm for training graduate students interested in neuroscience and computation. 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. The Computational Neuroscience Program is funded in part by a National Science Foundation Integrative Graduate Education and Research Traineeship (IGERT) grant. The Executive Committee consists of Timothy J. Ebner, Neuroscience, and Donald G. Truhlar, Supercomputing Institute Director, Chemistry, Chemical Physics, and Scientific Computation.

Partnerships

Computational Life Sciences Program

The Computational Life Sciences Program is an initiative of the University of Minnesota Supercomputing Institute that is intended to foster the growth of research in computational biology. To do this, the Supercomputing Institute has entered into a special partnership with IBM, which provides the following mutual benefits:

- IBM receives feedback through personal communications of user support and systems staff and through the Supercomputing Institute's research report series.
- University of Minnesota/IBM partnership activities with researchers, including joint efforts with affiliates, are fostered.
- The Supercomputing Institute provides a specially focused program for meeting needs of the entire University of Minnesota high-performance computing research community and the emerging computational needs of the biology community.
- Both IBM and the University benefit from the development of the software expertise needed to take advantage of IBM's DB2 and DiscoveryLink software.
- IBM staff members have offices at the Supercomputing Institute, which increases the opportunities for partnership interactions.

IBM has awarded the Supercomputing Institute several Shared University Research (SUR) grants, which promote this initiative.

This initiative also includes an affiliates program that provides an opportunity for Minnesota industry and other Minnesota research institutions with interests in the area of computational biology to have access to these computational resources, software, and technical support. The current affiliates are Cargill, the Hormel Institute, and the Mayo Medical School.

Further information about this program is available at:
http://www.msi.umn.edu/general/Programs/uofmibm/index.html

Partnerships (continued)

Laboratory for Computational Science and Engineering

The Supercomputing Institute partners with the Laboratory for Computational Science and Engineering (LCSE). 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 online data sets, particularly if they must be accessed at very high bandwidth, and applications requiring very high-resolution visualizations, particularly if image animations are needed. Distributed computing applications with tight coupling of computing resources on a fast network are also encouraged.

This partnership was overseen and guided during 2002–03 by the following committees:

Executive Committee

Donald G. Truhlar, Supercomputing Institute Director, Chemistry, Chemical Physics, and Scientific Computation

Paul R. Woodward, Astronomy and Scientific Computation

Program Committee

Paul R. Woodward, Astronomy and Scientific Computation, *chair*

David A. Yuen, Geology and Geophysics and Scientific Computation

Minnesota Health Informatics Seminar Series

The Supercomputing Institute, along with the Digital Technology Center, co-sponsored a series of seminars for the Graduate Program in Health Informatics at the University of Minnesota in Fall 2002. Speakers from the University of Minnesota, other research institutions, government, and industry gave presentations on a variety of topics from the health informatics field. Some individual seminars were also sponsored by the Biotechnology Institute or the Mathematics Colloquium. The symposium series was organized by Lynda Ellis, Department of Laboratory Medicine and Pathology. Non-University speakers included representatives from the Minnesota Department of Health, the Mayo Clinic, Minnetronix, Incorporated, and LHASA, Ltd.

Research Scholarship Program

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 that 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 partial support of research associates who work closely with Supercomputing Institute principal investigators on their research projects. Over the past 11 years, 180 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.

During 2002–03 the Supercomputing Institute awarded research scholarships to:

Titus V. Albu, Department of Chemistry

Vittorio Cristini, Department of Mathematics, Institute for Mathematics and Its Applications

Dacian Daescu, Institute for Mathematics and Its Applications

Fabien Dubuffet, Department of Geology and Geophysics

Serkan Erdin, Texas A&M University, College Station, Texas

Giuseppe Fadda, University of Padua, Padua, Italy

William Herb, Department of Civil Engineering, St. Anthony Falls Laboratory

Emmanuel Lorin de la Grandmaison, CEA/DAM Ile-de-France, Bruyere-le-Chatel, France

Leeor Kronik, Department of Chemical Engineering and Materials Science

Xabier Lopez, University of the Basque Country, Spain

Hisao Nakamura, Department of Chemistry

Yuri Nesmelov, Department of Biochemisty, Molecular Biology, and Biophysics

Tina Poulsen, Department of Chemistry

Joseph Resovsky, Department of Geology and Geophysics

Dongsu Ryu, Chungnam National University, Daejun, Korea

Venugopal Vuruputur, Center for Ocean-Land-Atmosphere Studies, Calverton, Maryland

Hong Wang, Department of Civil Engineering, St. Anthony Falls Laboratory

Research Scholarship Peer Review Panel for 2002–03

Graham V. Candler, Aerospace Engineering and Mechanics and Scientific Computation, *chair*

Leonard J. Banaszak, Biochemistry, Molecular Biology, and Biophysics

David J. Lilja, Electrical and Computer Engineering and Scientific Computation

John S. Lowengrub, Mathematics and Scientific Computation

Yousef Saad, Computer Science and Engineering and Scientific Computation

J. Ilja Siepmann, Chemistry and Scientific Computation

Undergraduate Internship Program

The Supercomputing Institute provides an Undergraduate Internship Program for undergraduate students throughout the country. The focus of the program is the application of computational approaches and visualization methods to supercomputing research. 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. Faculty from various disciplines have contributed projects and supervise the undergraduate students in their daily work. This program provides an opportunity for a challenging and enriching educational experience for undergraduate students interested in pursuing graduate or professional education. The program has sponsored 428 interns in its 13 years of existence.

The Supercomputing Institute awarded internships to the following undergraduates for Summers 2001 and 2002:

Anthony Anderson, University of Minnesota

Abdul Bahar, University of Minnesota

Victoria Bedell, Bethel College

Sarah Betterman, University of Minnesota

Nenad Bjelorglic, University of Minnesota

Adam Butensky-Bartlett, Northwestern University

Michael Garrels, Case Western Reserve University

Jerome Hauser, Princeton University

Peter Holm, Iowa State University

Eric Johnson, University of Minnesota

Christopher Kauffman, University of Minnesota

Elmer Kim, Harvey Mudd College

Jennifer Klein, College of St. Benedict

Benjamin Langmead, Columbia University

Margot LeClair, Haverford College

Peter Mack, St. John's University

Daniel Melendez, Universidad Metropolitana, Bayamon, Paraguay

John O'Leary, University of Chicago

Mariah Olson, University of Minnesota

Nick Olson, University of Maryland

Jonathan Othmer, Williams College

William Ryan, Rice University

Sosheel Saleem, University of Houston

Dawn Schafer, Bethel College

Justin Sjulson, University of Minnesota

Samuel Stechmann, University of Saint Thomas

Michael Tobin, Macalester College

Mychel Varner, Truman State University

Sterling Greg Williams, University of Minnesota

Hiu L. (Amy) Wong, University of North Carolina–Chapel Hill

Undergraduate Internship Committee for 2002–03

William B. Gleason, Laboratory Medicine and Pathology, *chair*

David D. Thomas, Biochemistry, Molecular Biology, and Biophysics and Scientific Computation

Donald G. Truhlar, Supercomputing Institute Director, Chemistry, Chemical Physics, and Scientific Computation

Fellows of the Institute

Fellows

Douglas N. Arnold
Daniel L. Boley
Graham V. Candler
James R. Chelikowsky
Bernardo Cockburn
Christopher J. Cramer
H. Ted Davis
Philippe de Forcrand (adjunct)
Jeffrey J. Derby
David H. Du
David M. Ferguson
Efi Foufoula-Georgiou
Jiali Gao
William B. Gleason
Alexander Y. Grosberg
J. Woods Halley
Dennis A. Hejhal
Thomas W. Jones
Daniel D. Joseph
Thomas H. Kuehn
Vipin Kumar
David J. Lilja
John S. Lowengrub
Mitchell B. Luskin
Alon V. McCormick
Douglas H. Ohlendorf
Hans G. Othmer
Suhas V. Patankar
J. Ben Rosen
Yousef Saad
L. E. Scriven
George R. Sell
J. Ilja Siepmann
Charles C. S. Song
Kumar K. Tamma
David D. Thomas
Donald G. Truhlar
Oriol T. Valls
Renata M. Wentzcovitch
George L. Wilcox
Paul R. Woodward
David A. Yuen

Associate Fellows

Leonard J. Banaszak
Charles E. Campbell
Robert W. Carr
Cynthia A. Cattell
Jane H. Davidson
Roger L. Fosdick
Sean C. Garrick
William W. Gerberich
Steven L. Girshick
Richard J. Goldstein
Anand Gopinath
Gautam Gowrisankaran
Satish C. Gupta
Bojan Guzina
Jerome F. Hajjar
Franz Halberg
Shaul Hanany
Joachim V. Heberlein
John R. Hiller
Wei-Shou Hu
Steven R. Kass
Paul Kiprof
Katherine Klink
Uwe R. Kortshagen
Joseph F. Labuz
James R. Leger
Perry H. Leo
Kenneth R. Leopold
David G. Levitt
Robert L. Lysak
Christopher W. Macosko
Peter H. McMurry
Fernando Porté-Agel
David Y. H. Pui
Shri Ramaswamy
P. Paul Ruden
Lanny D. Schmidt
Terrence W. Simon
Friedrich Srienc
Heinz G. Stefan
Henryk K. Stolarski
Robert T. Tranquillo
Randall H. Victora
Vaughan R. Voller

National Advisory Board

The National Advisory Board, made up of national experts in several areas of high-performance computing, had three members in 2002:

Dr. David Keyes, Lawrence Livermore National Laboratory

Professor Steven Louie, University of California, Berkeley

Professor Robert W. MacCormack, Stanford University

Administrative Staff

Director	Donald G. Truhlar
Research Programs Administrator and Assistant to the Director	Kay Anderson
Executive Administrative Specialist	Tracey Bartlett
Executive Administrative Specialist	Jessica Dziewecynski
Executive Administrative Specialist	Annice Larkin
Executive Administrative Specialist	Barbara Opal
Secretarial Assistant	Angie Reid
Webmaster	Shyam Boriah
DTC Assistant Director for Human Resources	Ann Johns
DTC/MSI Senior Accountant	Brian Carlton
DTC/MSI Principal Accounts Assistant	Jennifer Harrison
DTC/MSI Principal Administrative Specialist and Receptionist	Marni Anderson

Technical Support Staff

Manager of Systems, Operations, and User Support	Barry Schaudt

Scientific Computation User Support Specialists

Basic Sciences Laboratory Manager, Computational Chemistry and Biochemistry Consultant	Patton Fast
Scientific Computation Consultant, User Support Group Leader	Birali Runesha
Medicinal Chemistry Visualization–Workstation Manager, Computational Biology/Biochemistry Consultant	Yuk Sham
Computational Biology Consultant	Zheng Jin Tu
Computational Genomics Consultant	Wayne Xu
Scientific Development and Visualization Lab Manager, Scientific Computation Consultant	Shuxia Zhang

Operations Staff

UNIX Systems Administrator	Shawn Amundson
UNIX Systems Administrator	Dack Anderson
Assistant Network Administrator	Ben Beuchler
Systems Support Technician	John Boggs
IBM SP System Administrator	Kirk Deen
Web Interface Programmer	Wen Dong
Lead Windows/Mac Administrator	Richard Flesvig
UNIX Systems Administrator	Yectli Huerta
Tape Backup/UNIX Systems Administrator	Thomas Kniffen
LINUX Cluster/UNIX Systems Administrator	Ben Kochie
Windows/Mac Administrator	Paul Lammert
Lead Network Administrator	Samantha Thomas
SGI Origin Systems Administrator	Gabe Turner

Committee and Panel Members 2002–2003

Yusuf J. Abul-Hajj, Medicinal Chemistry
Leonard J. Banaszak, Biochemistry, Molecular Biology, and Biophysics
Judith G. Berman, Genetics, Cell Biology, and Development
Daniel L. Boley, Computer Science and Engineering and Scientific Computation
Graham V. Candler, Aerospace Engineering and Mechanics and Scientific Computation
Cynthia A. Cattell, Physics and Astronomy
James R. Chelikowsky, Chemical Engineering and Materials Science and Scientific Computation
Bernardo Cockburn, Mathematics and Scientific Computation
Christopher J. Cramer, Chemistry and Scientific Computation
Jeffrey J. Derby, Chemical Engineering and Materials Science and Scientific Computation
Fred Dulles, Coordinator of Information Technology, College of Biological Sciences
Jiali Gao, Chemistry and Scientific Computation
Sean C. Garrick, Mechanical Engineering
William B. Gleason, Laboratory Medicine and Pathology
David J. W. Grant, Pharmaceutics
Alexander Y. Grosberg, Physics and Astronomy and Scientific Computation
Satish C. Gupta, Soil, Water, and Climate
Ashley T. Haase, Microbiology
Jerome F. Hajjar, Civil Engineering
Rodney L. Johnson, Medicinal Chemistry
Thomas W. Jones, Astronomy and Scientific Computation
Vivek Kapur, Veterinary Pathobiology
George Karypis, Computer Science and Engineering and Scientific Computation
Steven R. Kass, Chemistry
Yiannis Kaznessis, Chemical Engineering and Materials Science
Arkady Khodursky, Biochemistry, Molecular Biology, and Biophysics
Daniel M. Kroll, Pharmacy and Scientific Computation
Vipin Kumar, Computer Science and Engineering and Scientific Computation
David J. Lilja, Electrical and Computer Engineering and Scientific Computation
David H. Live, Biochemistry, Molecular Biology, and Biophysics
John S. Lowengrub, Mathematics and Scientific Computation
Mitchell B. Luskin, Mathematics and Scientific Computation

Continued on next page

Committee and Panel Members 2002–2003 (continued)

Krishnan Mahesh, Aerospace Engineering and Mechanics

Kevin H. Mayo, Biochemistry, Molecular Biology, and Biophysics

Alon V. McCormick, Chemical Engineering and Materials Science

Gary W. Meyer, Computer Science and Engineering

Douglas H. Ohlendorf, Biochemistry, Molecular Biology, and Biophysics

Michael J. Olesen, Digital Technology Center

Hans G. Othmer, Mathematics and Scientific Computation

Ronald L. Phillips, Agronomy and Plant Genetics

Yousef Saad, Computer Science and Engineering and Scientific Computation

J. Ilja Siepmann, Chemistry and Scientific Computation

Friedrich Srienc, Biotechnology Institute and Chemical Engineering and Materials Science

Henryk K. Stolarski, Civil Engineering

David D. Thomas, Biochemistry, Molecular Biology, and Biophysics and Scientific Computation

Donald G. Truhlar, Supercomputing Institute Director, Chemistry, Chemical Physics, and Scientific Computation

Randall H. Victora, Electrical and Computer Engineering

Vaughan R. Voller, Civil Engineering and Scientific Computation

Lawrence P. Wackett, Biochemistry, Molecular Biology, and Biophysics

Carston R. Wagner, Medicinal Chemistry

Kylie J. Walters, Biochemistry, Molecular Biology, and Biophysics

Jon B. Weissman, Computer Science and Engineering

Renata M. Wentzcovitch, Chemical Engineering and Materials Science

Martin W. Wessendorf, Neuroscience

George L. Wilcox, Neuroscience and Scientific Computation

Carrie M. Wilmot, Biochemistry, Molecular Biology and Biophysics

Paul R. Woodward, Astronomy and Scientific Computation

Darrin M. York, Chemistry and Scientific Computation

David A. Yuen, Geology and Geophysics and Scientific Computation

External Support

Principal Investigator	Source of Funding
Roger E. A. Arndt	National Science Foundation Office of Naval Research
Leonard J. Banaszak	National Institutes of Health National Science Foundation
George Barany	National Institutes of Health
Avram Bar-Cohen	Fluent/Icepack Sony ITC
Victor H. Barocas	National Science Foundation Sandia National Laboratories Whitaker Foundation
Bridgette A. Barry	National Institutes of Health National Science Foundation
Judith G. Berman	National Institute of Dental and Craniofacial Research National Institutes of Health
John C. Bischof	National Institutes of Health Urologix, Inc.
David A. Blank	American Chemical Society National Science Foundation
Bruce R. Blazar	National Institutes of Health
Victor A. Bloomfield	National Institutes of Health
Charles E. Campbell	Office of Naval Research
Stephen A. Campbell	BH Electronics National Science Foundation Semiconductor Research Corporation/IBM Semiconductor Research Corporation/Motorola Semiconductor Research Corporation/SEMATECH
Graham V. Candler	Air Force Office of Scientific Research National Aeronautics and Space Administration National Science Foundation
Robert W. Carr	National Aeronautics and Space Administration National Science Foundation
Cynthia A. Cattell	National Aeronautics and Space Administration Research Corporation
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Continued on next page

External Support (continued)

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Robert F. Cook	Industrial Partnership for Research in Interfacial and Materials Engineering
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Steven L. Girshick	Army Research Office National Science Foundation
Wayne L. Gladfelter	National Science Foundation
Richard J. Goldstein	Advanced Gas Turbine System Research

External Support (continued)

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Rolf Grütter	National Institutes of Health
John S. Gulliver	Army Corp of Engineers
Satish C. Gupta	Corn Council Legislative Commission on Minnesota Resources Soybean Council
Bojan Guzina	National Science Foundation Minnesota Department of Transportation
Franz Halberg	Colin Medical Instruments Earl Bakken Fund Fukuda Denshi National Institutes of Health
J. Woods Halley	Department of Energy National Science Foundation
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Kristin A. Hogquist	National Institutes of Health
Raymond M. Hozalski	Strategic Environmental Research and Development Program
Rodney L. Johnson	National Institutes of Health

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External Support (continued)

Principal Investigator	Source of Funding
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Daniel D. Joseph	Department of Energy National Science Foundation
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Vipin Kumar	Army Research Laboratories Army Research Office Department of Energy National Aeronautics and Space Administration National Science Foundation
Joseph F. Labuz	National Science Foundation
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Robert L. Lysak	National Aeronautics and Space Administration
Chris Macosko	Army Research Office

External Support (continued)

Principal Investigator	Source of Funding
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Hiroshi Matsuo	Minnesota Medical Foundation
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Richard B. McClurg	3M
Alon V. McCormick	Industrial Partnership for Research in Interfacial and Materials Engineering
Ned Mohan	Office of Naval Research
David C. Morse	American Chemical Society National Science Foundation
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Michael P. Murtaugh	United States Department of Agriculture
Karin M. Musier-Forsyth	National Institutes of Health
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Yuan-Ping Pang	Defense Advanced Research Projects Agency National Institutes of Health Department of Veterans Affairs
James S. Pankow	National Institutes of Health
Ronald L. Phillips	National Science Foundation
Christopher A. Pennell	National Institutes of Health
Fernando Porté-Agel	National Aeronautics and Space Administration National Science Foundation
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David Y. H. Pui	Department of Energy
Shri Ramaswamy	Department of Energy Hercules, Inc.
Aaron David Redish	National Institutes of Mental Health

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External Support (continued)

Principal Investigator	Source of Funding
Jean F. Regal	Department of Defense
Fernando L. Reitich	Air Force Office of Scientific Research Army Research Office National Science Foundation
Ernest F. Retzel	National Science Foundation United States Department of Agriculture
P. Paul Ruden	National Science Foundation Office of Naval Research
Yousef Saad	Army Research Office National Science Foundation
Peter Santi	National Institute on Deafness and Other Communication Disorders
Arnd Scheel	National Science Foundation
Lanny D. Schmidt	Department of Energy National Science Foundation
L. E. Scriven	Industrial Partnership for Research in Interfacial and Materials Engineering National Science Foundation
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Robert W. Sterner	Fish and Wildlife Service
Henryk K. Stolarski	Local Road Research Board National Science Foundation Minnesota Department of Transportation

External Support (continued)

Principal Investigator	Source of Funding
Stanley A. Thayer	National Institutes of Health National Science Foundation
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Donald G. Truhlar	Department of Defense Department of Energy National Science Foundation
Oriol T. Valls	American Chemical Society
Randall H. Victora	Information Storage Industry Consortium National Science Foundation Samsung
Carston R. Wagner	National Institutes of Health
Kylie J. Walters	American Cancer Society Minnesota Medical Foundation
Dong Wang	Dow Agrosciences
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George L. Wilcox	National Institute on Drug Abuse National Science Foundation Pierre Fabre Research Institute Solvay Pharmaceuticals
Carrie M. Wilmot	Minnesota Medical Foundation National Institutes of Health
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Darrin M. York	American Chemical Society National Institutes of Health
Nevin D. Young	Department of Agriculture Plant Molecular Genetics Institute
David A. Yuen	Department of Energy National Science Foundation
Michael R. Zachariah	Defense Advanced Research Projects Agency National Science Foundation United States Army

Sponsored Symposia

Visual Processing of Natural Images: Theory, Psychophysics, Physiology, and Imaging

April 5–6, 2002

This conference, co-sponsored with the Computational Neuroscience Program, brought together interdisciplinary research representing theoretical, neurophysical, brain imaging, and psychophysical approaches to the problem of visual processing of natural images. The key goals of the conference were the discussion of the bridge between simple and complex (natural) images and extensions of the information theoretic perspective to understanding higher-level visual processing.

Sponsors

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Organizers

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Tom Carlson, University of Minnesota

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Patty Costello, University of Minnesota

Sheng He, University of Minnesota

Gordon Legge, University of Minnesota

Thomas Naselaris, University of Minnesota

Cheryl Olman, University of Minnesota

Paul Schrater, University of Minnesota

Computational Chemistry at the Interface

June 3–4, 2002

As part of the 34th Great Lakes Regional Meeting of the American Chemical Society, the Supercomputing Institute co-sponsored a mini-symposium on Computational Chemistry at the Interface. The mini-symposium featured sessions on the computational chemistry of nanostructured materials, environmental chemistry, and chemical biology.

Organizers

Donald G. Truhlar, University of Minnesota, *chair*

Christopher J. Cramer, University of Minnesota

Jiali Gao, University of Minnesota

Alon V. McCormick, University of Minnesota

Nanosimulation Workshop

August 26, 2002

The First Annual Nanosimulation Workshop was held at the University of Minnesota's Twin Cities campus on August 26, 2002. It was jointly sponsored by the Supercomputing Institute and the Center for NanoEnergetics Research (CNER). CNER is a research center created in the spring of 2001 at four university sites through the Department of Defense–University Research Initiative for NanoTechnology (DURINT). The Univeristy of Minnesota is the lead institution; the others are the University of Delaware, Oklahoma State University, and South Dakota School of Mines and Technology. The talks included presentations by CNER researchers and complementary research by a distinguished group of invited speakers. The workshop organizer was Donald G. Truhlar, University of Minnesota.

More Information

For more information on past and future symposia sponsored in part by the Supercomputing Institute, please refer to our Internet pages at:

www.msi.umn.edu/general/events.html

Ongoing and Recently Completed Research Projects

January 1, 2002—March 15, 2003

University of Minnesota—Duluth

College of Science and Engineering

School of Medicine

Paul Kiprof, Associate Fellow

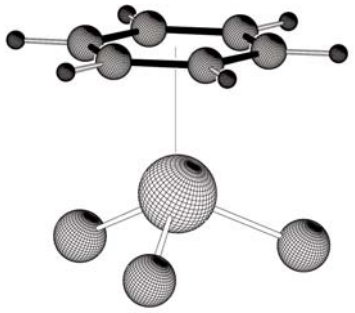
High-Valent Transition Metal Arene Complexes and Carboxonium Ions

This research project involves two major areas: the study of high-valent transition metal arene complexes, and the study of the stability of rearrangement of carbocations.

Transition metal complexes where the metal is in a high oxidation state are rare and theoretically not well described. This project complements synthetic work in this area with theoretical calculations that address the issue of bonding of the arene to the transition metal fragment. Commonly the bonding in transition metal arene complexes is explained as a combination of two classes of orbital interactions. Firstly, filled orbitals of the benzene (or arene) π system interact with empty orbitals in the transition metal (referred to as "bonding" or "donation"). Secondly, filled orbitals of the transition metal interact with empty orbitals of the arene (referred to as "backbonding" or "backdonation").

In the case of transition metal fragments that are in a high oxidation state, the bonding only relies on the first part, making the complexes much less stable than their well-known low-valent counterparts. During this research period, this group has made progress in calculating the structures and energies of the low-valent comparison structures. They have also begun calculations to describe the exchange of arene complexes, which uniquely happens at low temperatures in these cases. They have identified a viable intermediate and are further investigating it.

The second part of this project is concerned with the effects that heteroatoms have on the stability and chemistry of carbocations. Oxygen substituents typically stabilize carbocations through the formation of π bonds. Therefore, these carboxonium ions can achieve stability under normal, preparative conditions, which makes them interesting for synthetic applications. The researchers have studied several cage cations, and are moving to unrestrained structures that have more conformational flexibility. They are also extending their research to heteroatoms other than oxygen, in order to compare their effects versus that of oxygen.



Calculated structure of the benzene complex of $TiCl_3^+$.

In related research using the Basic Sciences Computing Laboratory, these researchers are studying the reaction of silicon-carbon double bonds with other molecules that have multiple bonds. In particular, they are studying the reaction of silene and ethylene. This reaction was discovered recently and poses a challenge to the understanding of cycloaddition reactions. In the case of pure carbon compounds, these reactions are known to proceed photochemically, whereas the reactions involving silicon proceed thermally and can be carried out in the dark. The transition state of the silene reactions in the concerted type of this reaction have already been studied. The current research is concerned with alternative stepwise pathways of the reaction that involve stable intermediates.

Research Group

Beau Barker, Graduate Student Researcher
Melissa Frank, Undergraduate Student Researcher
Dimitry Litvinov, Graduate Student Researcher
Carl Sandness, Graduate Student Researcher

Ted Pedersen, Principal Investigator

Word Sense Disambiguation in High-Dimensional Feature Space

Most words in natural language have multiple possible meanings. This simple fact causes no end of difficulties for computer systems that seek to understand human language. The goal of this project is to develop computational methods that automatically determine which meaning of a word is intended in a particular context, and easily adapt to the variations in word meaning that accompany changes in the subject matter and intended audience of a text. Word meanings are central to language understanding, and success in this research will improve the ability of computer systems to perform translation, retrieve information from the World Wide Web, and summarize documents.

Research Group
Amruta Purandare, Graduate Student Researcher

Masha Sosonkina, Principal Investigator

Enabling Environments for High-Performance Computing

Modern scientific applications demand computing power on the order of trillions of operations per second. Rapid advances in processor, memory, and interconnection technologies have brought about the era of wide-area performance distributed computing. However, most applications using these distributed systems achieve only a fraction of the peak aggregate performance of the underlying hardware and middleware. The Grid is a new computing paradigm that aims to provide a seamless uniform access to heterogeneous distributed resources. To make effective use of the Grid, it is critical that applications and supporting tools have a seamless interface with Grid services, dynamically adapt to changes in the heterogeneous resources, and are able to scale. In particular, the heterogeneity of communication resources poses a major problem for adapting scientific applications, which are typically characterized by a set of computational tasks and in which data communications are considered a parallel overhead. In addition, the scientific application user/developer is typically not trained in the network programming required for monitoring the performance of the communication channels.

The goal of this research is twofold: to achieve transparent tuning of high-performance applications to the communication subsystem while facilitating transition to future programming models, and to augment the newly developed and enhanced programming models with information about the communication environment. The project focuses on providing communication middleware that enables runtime communication support for high-performance applications and provides a seamless interface to a variety of programming and application development environments.

Research Group and Collaborator
Devdatta Kulkarni, Graduate Student Researcher
Yousef Saad, Faculty Collaborator
Samuel Storie, Graduate Student Researcher

John R. Hiller, Associate Fellow

Nonperturbative Analysis of Field Theories Quantized on the Light Cone

This project involves quantum field theories, which are the standard means for formulating interactions between fundamental particles. When written in terms of light-cone coordinates, where c is the speed of light, z is the spatial coordinate, t is real time, and $ct+z$ plays the role of time, such theories can be easier to solve numerically. Many difficulties remain, however, one of them being the existence of infinities associated with couplings to modes of arbitrarily large energies. This project explores two different methods for the removal of such infinities. One is known as Pauli-Villars regularization, in which additional particles are added to the theory, with interactions and norms chosen to achieve the desired cancellations. The masses of these Pauli-Villars particles are kept large enough not to influence the physics of interest at low energies. The other approach is to consider supersymmetric theories where the cancellation can be automatic, and where the difficulty becomes that of removing unwanted particles from the low-energy physics by carefully breaking the supersymmetry.

This researcher has completed an application of an improved Pauli-Villars regularization scheme to an analytically soluble truncation of Yukawa theory. This represents a point of comparison for numerical calculations now in progress that include more particles in the basis. Of particular interest will be the relative probabilities of these many-particle states as functions of the coupling strength and Pauli-Villars masses. To support this numerical calculation, the code has been significantly revised. It now uses an order of magnitude more Lanczos iterations, combined with an automated restarting of the iterations, because improved convergence of the eigenvalue problems was found to be critical for rapid and successful solution of the renormalization conditions. The increase in iteration count required alteration of the Lanczos algorithm to avoid disk storage of intermediate vectors. This not only eliminates the storage requirement but also the overhead for disk input/output at the cost of repeating the Lanczos iterations to construct the eigenvector once the physical ground state has been selected.

In the work on supersymmetric Yang-Mills (SYM) theory, a Chern-Simons (CS) term has been added to provide an effective mass for the constituents without breaking the supersymmetry. Studies of the SYM-CS theory have been completed for 1+1 and 2+1 dimensions. In 2+1 dimensions, the sites of the matrices became large enough to require supercomputing resources. The effective mass introduced by the CS term had the desired effect of reducing the average number of constituents for all but the strong-coupling regime of the (2+1)-dimensional theory. The reduced number of constituents improves the applicability of the underlying discretization of the field theory. The masses and wave functions of the eigenstates were analyzed, including those with excitations of transverse modes. Such modes are the analog of experimental signals for higher dimensions. Other particularly interesting states are those connected to massless states in the pure SYM theory. The CS term gives them mass, but the masses are nearly independent of the SYM coupling. This may be a new mechanism for generating states of a theory that are much lighter than the natural energy states. The work has since been extended to include the analog of quark fields and their superpartners, in order to build eigenstates resembling the mesons of the standard strong-interaction theory, quantum chromodynamics.

Lester R. Drewes, Principal Investigator

Microarray Analysis of Blood-Brain Transport and Metabolism

The metabolic energy required for brain function under most circumstances is derived from the oxidation of the simple blood sugar, glucose. However, during early development, long-term fasting, high fat/low carbohydrate diet, and hibernation, the brain uses ketone bodies as alternative fuels. It is thought that this metabolic adaptation occurs as a result of altered protein and gene expression in the cells of the blood–brain barrier and of the brain parenchyma.

These researchers are using oligonucleotide (Affymetrix) and carrier deoxyribonucleic acid (cDNA) arrays to analyze gene expression profiles of brain microvessels and brain tissue from animals (rat, mouse, ground squirrel) under different experimental conditions. For example, samples from animals on a control diet will be compared to those from a ketogenic diet and samples at different postnatal ages will be compared to adult samples. Finally, samples from brain following an experimental stroke will be compared to normal tissue to examine pathophysiological processes and possible neuroprotection by altered brain substrates. The results may provide insight into mechanisms of blood–brain transport, pathways of metabolism, and possible neuroprotective treatments or strategies.

Research Group
Brad Enerson, Graduate Student Researcher

Jean F. Regal, Principal Investigator
Ronald R. Regal, Co-Principal Investigator

Differential Allergen Sensitivity in Asthma in Young and Adult Mammals

The objective of this research is to determine if young and adult animals differ in their sensitivity to allergens, both in the induction phase of asthma as well as in elicitation of the asthma symptoms. Besides examining pulmonary function and inflammation in the lung, this project examines gene expression in the lungs of both young and adult animals to determine if differences can be identified in the mechanism of asthma depending on age and gender. Molecular differences discovered in different asthma phenotypes may provide information regarding appropriate therapy for the disease depending on the age and gender of the individual.

The group is using the resources of the Computational Genetics Laboratory to assist in analysis of the gene expression data.

Research Group and Collaborator
Amy Greene, Research Associate
Mark Rutherford, Faculty Collaborator

University of Minnesota—Hormel Institute

Hormel Institute

Zigang Dong, Principal Investigator

Signal Transduction in Cancer Development

Signal transduction plays an important role in cancer development. These researchers are investigating the key signals in cancer development with the goal of finding a way to block the signals. This could then be used as a tool for cancer prevention.

Research Group

Feng Zhu, Research Associate

University of Minnesota—Twin Cities

College of Agricultural, Food, and Environmental Sciences

Department of Agronomy and Plant Genetics

Department of Animal Science

Department of Plant Pathology

Department of Soil, Water, and Climate

College of Biological Sciences

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St. Anthony Falls Laboratory

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Department of Electrical and Computer Engineering

Department of Geology and Geophysics

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Institute for Mathematics and Its Applications

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Department of Neuroscience

Department of Neurosurgery

School of Dentistry

Department of Diagnostic/Surgical Sciences

Department of Oral Sciences

Department of Preventative Sciences

School of Public Health

Division of Environmental and Occupational Health

Division of Epidemiology

James A. Anderson, Principal Investigator

In Silico Mapping of Wheat

Fusarium head blight (FHB) is one of the most destructive diseases of wheat worldwide. These researchers have identified a major quantitative trait locus (QTL) for FHB resistance, located on the wheat chromosome 3BS. Their objective is to identify wheat expressed sequence tagged sites (ESTs) located in this major QTL region. More than 140,000 wheat ESTs were deposited in GenBank by the end of April 2002, so it is impractical to map such a large number of wheat ESTs by Southern blotting. The researchers are taking advantage of the synteny between wheat chromosome 3B and rice chromosome 1 to identify wheat ESTs in this major PTL region via an *in silico* mapping strategy which compares rice chromosome 1 to the wheat EST database.

Research Group

Sixin Liu, Research Associate
Susan Reynolds, Graduate Student Researcher
Emily Wennerlind, Research Associate

Ronald L. Phillips, Principal Investigator
Howard W. Rines, Co-Principal Investigator

Chromosomal Distribution of Maize Repetitive Sequences

This group uses microarray technology in conjunction with labeled deoxyribonucleic acid (DNA) from oat-maize addition (OMA) lines to perform chromosomal analysis of the organization and distribution of maize repetitive elements. Each OMA line contains an individual maize chromosome allowing for an analysis of its composition. The probes in this research were specifically designed to detect unique motifs of repetitive sequences or whole elements. This microarray technology is a fluorescence comparative assay using differently labeled genomic DNA from OMA lines hybridized to immobilized probes. Target sequences are quantified for their relative abundance per chromosome. In addition, fluorescence *in situ* hybridization (FISH) is used to show the physical distribution of the major elements along a maize chromosome. Microarray and FISH techniques together elucidate specific repetitive elements within a maize chromosome, clarify genomic organization, and can reinforce chromosome duplication models.

Research Group

Wade Odland, Graduate Student Researcher

David A. Somers, Principal Investigator

Characterization of Transgene Loci

These researchers are using the resources of the Basic Sciences Computing Laboratory to analyze the genome scale to determine whether transgene integration sites correspond to various sequence motifs. Among these are palindromes, purine-pyrimidine stretches, matrix-attachment regions, topoisomerase binding sites, and other deoxyribonucleic acid-binding sites.

Research Group
Rachel Mann, Graduate Student Researcher

Yang Da, Principal Investigator

Graphical Visualization of Gene Flows in Large Complex Pedigrees

Graphical pedigree visualization of gene flows in a population is helpful for identifying the genetic trend of a characteristic and for selecting an optimal population structure for gene mapping. However, such graphical visualization is tremendously difficult in large complex pedigrees. Recently, this researcher has developed the "Pedigraph" computer program to implement the task of graphical visualization of these pedigrees; initial tests of the program have been successful. The researcher is now testing the feasibility of the Pedigraph program for large cattle populations and to identify the genetic trait of female fertility, a difficult problem facing the dairy industry. Several million records, at least, must be processed. This huge amount of data and the computationally intensive graphic displays necessitate the use of the supercomputers.

Scott C. Fahrenkrug, Principal Investigator

Vertebrate Comparative and Functional Genomics for Medical and Agricultural Research

These researchers are developing a database to facilitate the integration of physical and genetic data from human, mouse, zebrafish, and livestock genomes. This database will allow for collection, storage, and analysis of genetic and sequence data from these species and will allow for the identification of regions of conserved synteny. This conserved synteny, as well as phenotypic and gene-expression data, will be used to functionally annotate vertebrate genes. This ability will allow the design of experiments to address the function of genes in processes of medical and agricultural importance.

Research Group
Yongqing Zhang, Graduate Student Researcher

Nevin D. Young, Principal Investigator

Patterns of Plant Gene Family Evolution

These researchers are investigating the mechanisms of evolution of large gene families in plant genomes. This involves inferring the evolutionary histories of a large number of gene families, both within single species and across multiple species, as well as making whole-genome comparisons to assess which genes have arisen through local duplications, large-scale genomic duplications, or other mechanisms. Several aspects of this project require substantial computing resources, including sequence alignments, calculations of phylogenetic trees (evolutionary histories), clustering of protein families, and whole-genome similarity comparisons.

Research Group and Collaborator
Steven Cannon, Graduate Student Researcher
Dana Larsen, Research Associate
Georgiana May, Faculty Collaborator
Joann Mudge, Research Associate

Satish C. Gupta, Associate Fellow

Quantifying Riverbank Erosion Using Airborne Scanning Laser Altimetry

The Minnesota River flows through a relatively flat agricultural landscape, but is fed by tributaries that are incised with steep and unstable stream banks. It is not clear what proportion of the sediment and nutrient pollution in the Minnesota River is from upland erosion vis-á-vis stream bank collapse. This study evaluated the feasibility of using an airborne scanning laser to estimate riverbank erosion. Specifically, this project used a helicopter-mounted Topeye laser system to construct detailed digital elevation models of a geologically active river valley twice on an annual basis. A 56-km length of the corrider of the Blue Earth River in Minnesota was scanned April 2001 and April 2002. The database includes X, Y, Z coordinates of laser return from the river valley plus return intensity. Distance between footprints on the ground was generally between 60 and 100 cm. A bare earth model for both scans was made by stripping vegetation laser returns. One-meter-square grids were constructed for each annual scan and differenced to determine volume change over time. The sum of grid cell differences was multiplied by average bank material bulk density to estimate mass wasting. The percentage of sediment in the river sourced from bank materials was determined as the proportion of mass wasting to sediment load measured at a downstream gauging station. The percentage of sediment from bank erosion varied from 23 to 56 depending on the range of textural material that is transportable once in the river. Based on analysis of riverbank samples, 201 tons/yr of materials comes from bank erosion and slumping.

Research Group

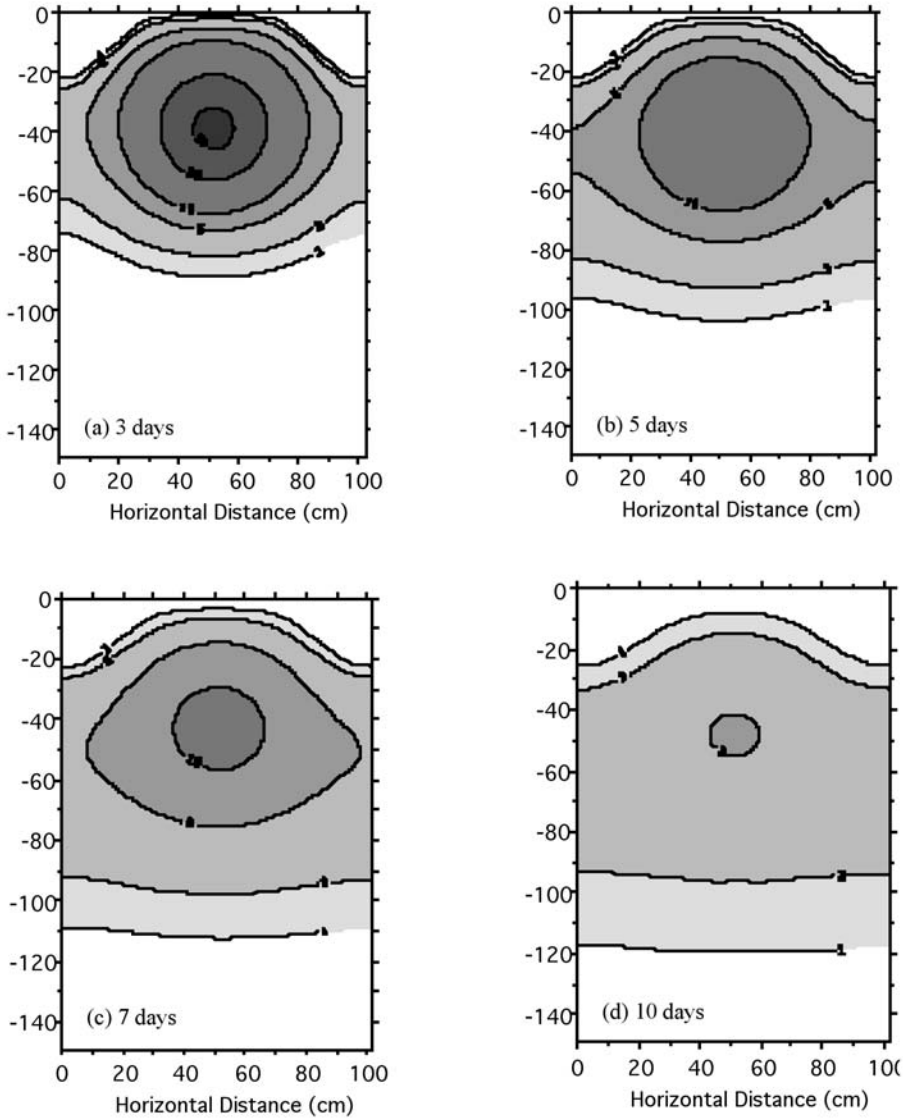
David Thoma, Graduate Student Researcher
Cal Kirchof, Staff

Riverbank sloughing along the Blue Earth River, Minnesota.

Dong Wang, Principal Investigator

Modeling Two-dimensional Fumigant Gas Transport in Subsurface Soils and Volatilization Into the Atmosphere

The dynamics of pesticide volatilization are strongly controlled by subsurface transport and ambient environmental conditions, which may be described with process-based transport models. Application of simulation models can provide accurate characterization of fate and transport of volatile organic chemicals such as 1,3-dichloropropene and chloropicrin and their concentration dynamics that may be used as an index for pest control efficacy. But many parameters are often required for these types of mathematical models that translate to the initial and boundary conditions. Selection of a combination of sets of parameters optimized for better distribution uniformity and the least volatilization loss has a very practical value for field application by pesticide specialists and farm managers. This project integrates an existing comprehensive two-dimensional pesticide simulation model with management selections by adopting the most efficient numerical schemes.



Spatial distribution of air-phase concentration of 1,3-D at (a) 3 days, (b) 5 days, (c) 7 days, and (d) 10 days after application at 30 cm depth in a sandy loam soil.

During this research period, the group made significant progress towards modifying a two-dimensional pesticide transport model to simulate the distribution and volatilization of soil fumigants when applied through subsurface drip irrigation. The program provides a database with default soil and chemical properties to predict subsurface distribution patterns and potential surface volatilization losses of soil fumigants under a selected field configuration and application regimes. Up to three chemicals can be simulated simultaneously. Physical and chemical properties of cis- and trans-isomers of 1,3-dichloropropene and chloropicrin for a typical medium-textured soil were given as default values in the model input. Properties of other soil fumigants can be substituted as input options during program initialization, if some or all the parameters are known from laboratory or field measure-

Continued on next page

Dong Wang, Principal Investigator

ments or other sources. A database containing hydraulic properties of twelve soil series (from clay to sand) were created as selectable sets of input values. Substitution is allowed if properties of an individual soil are known. The output includes a normalized run-time volatilization flux display and selections in post-processing. Output options from the post-processing program include data and graphs of cumulative volatilization loss, volatilization flux density, and concentration profile by time for a selected location or by location for a selected lapsed time after application.

Research Group

Jingming He, Research Associate
Kurt Spokas, Graduate Student Researcher
Hui L. (Amy) Wong, Supercomputing Institute Undergraduate Intern
Jindong Wu, Graduate Student Researcher

Arkady Khodursky, Principal Investigator

Transcriptional Dynamics of Complex Transitions

Growing cells cycle through overlapping stages of responses to internal and external cues. Some responses require concerted switching from the cycling routine. These researchers have shown that microarray analysis of messenger ribonucleic acid (mRNA) levels can be very useful in delineating such responses by determining transient changes in mRNA abundances, as well as transcripts' composition and levels corresponding to new steady-states. But even for well-established processes, the exact sequence of transcriptional events accompanying the process is not known. These researchers are using the Computational Genetics Laboratory to perform temporal sequencing of such events. This information will help them to understand the basis of regulation, pathway connectivity, and intracellular flow of information and the "logic" behind it.

Research Group

Betsy Martinez-Vaz , Graduate Student Researcher

Friedrich Srienc, Associate Fellow

Cell Growth Dynamics of Unicellular Organisms

This research group is using Supercomputing Institute resources for two projects. The first of these involves investigation into cell growth dynamics. Cell properties such as mass, protein content, deoxyribonucleic acid (DNA) content, and other components 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. These researchers developed a mathematical model to take into account the distributed and staged nature of cell growth. The model consists of a system of population balance equations, each describing a different stage of the cell cycle, and an ordinary integro-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 also used to solve the single-variable, single-staged model under conditions of changing substrate concentration. The researchers are now extending 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.

The second project uses elementary mode analysis to investigate biochemical networks. Evolution has supplied biological organisms with a highly coupled network of hundreds of enzyme-catalyzed reactions. Scientific advances like polymerase chain reaction (PCR) have provided means of altering the topography of these reaction networks. For instance, enzymatic activities can be blocked by disrupting certain genes, or new reactions can be introduced through the expression of recombinant genes. Analysis of native and recombinant networks has been simplified by a number of theoretical tools.

One such method is elementary mode analysis. An elementary mode is the simplest balanced combination of substrates, products, and reactions that enforces a no-accumulation restriction on internal metabolites. The analysis program METATOOL determines all possible balanced elementary modes for a given reaction network (Pfeiffer et al., 1999). Such results can give information on product formation pathways and can determine basic parameters like maximum theoretical yield. Large, highly branched networks with multiple products and substrates often have numerous elementary modes. Determining all possible modes for these systems can result in a significant computational burden, making the use of Supercomputing Institute resources necessary.

Research Group

Ross Carlson, Graduate Student Researcher
Natarajan Vijayasankaran, Graduate Student Researcher
Abdelqader Zamamiri, Graduate Student Researcher

Sarah E. Hobbie, Principal Investigator

Nitrogen Dynamics in Biodiversity, CO_2, and Nitrogen

Biodiversity, CO_2, and Nitrogen (BioCON) is a long-term field experiment currently being conducted at the University of Minnesota's Cedar Creek Natural History Area. The central objective of BioCON is to determine how the composition and diversity of plant species influence community and ecosystem responses to CO_2 and N, and how these interactions are mediated by microbial mutualists, herbivores, pathogens, decomposers, and higher trophic levels in the soil, including the consequences of these interactions for ecosystem C and N dynamics and for autotroph and heterotroph communities. CO_2, N, and species composition and diversity treatments collectively alter the quantity, quality, and heterogeneity of autotroph chemistry (i.e., net primary productivity, NPP) both directly (via physiology) and indirectly (by competitive shifts in plant composition). Changes in the amount and chemistry of NPP in turn affect the production, composition, diversity, and interaction of herbivores, decomposers, microbial mutualists, and microbivores, which can feed back to influence autotroph chemistry and performance, including NPP, by altering C and N dynamics.

Major unresolved questions include the role of intra- and inter-trophic level interactions in:

- C and N dynamics under changing CO_2 and N regimes.
- The role of plant species composition and diversity in ecosystem response to CO_2 and N.
- The fate of increased C that enters ecosystems under higher atmospheric CO_2.

These researchers are using resources in the Computational Genetics Laboratory to analyze a complex dataset from this experiment that currently encompasses 371 field plots with 5 years of data. These data are most accurately analyzed with a repeated measures analysis, which first requires a maximum likelihood comparison of approximately eleven covariance structures to find the best model.

Research Group

Jason West, Research Associate

Scott M. Lanyon, Principal Investigator

Phylogeny of the Passerine Birds

The avian order Passeriformes is one of the largest terrestrial vertebrate radiations. Testing alternative explanations for this remarkable radiation depends critically on analysis of morphological, molecular, behavioral, and ecological variation in conjunction with a thorough understanding of evolutionary relationships within the group. This project focuses on interpreting phenotypic variation among species of passerines in the context of phylogenies derived from molecular data. The researchers have examined this variation at a variety of hierarchical levels, from species within genera, through families within the order. The data sets they have gathered to infer the phylogeny of this group are large, including up to 350 taxa and 4 kilobases of deoxyribonucleic acid (DNA) sequence. Phylogenetic analysis of such large datasets is computationally challenging, especially using mode-based approaches (e.g., maximum likelihood). The researchers have been using simpler parsimony-based approaches, but even these can be limiting due to processor speed, bus speed, and memory capacity. The researchers have begun to implement parallel computing approaches, and for this reason are using the resources of the Computational Genetics Laboratory.

Research Group

F. Keith Barker, Research Associate

Georgiana May, Principal Investigator

Genome Studies in *Ustilago*, Corn, and Solanaceae

These researchers are conducting evolutionary studies in plant-pathogen interactions. Specifically, dynamics of the fungal interaction between *Ustilago maydis* (corn smut) and corn provide a model system to examine the genomic structure and evolution of genes involved in plant-fungal interactions. The purpose of these studies is to determine the role of genome evolution in the evolution of resistance in plants and the evolution of virulence in the pathogen.

In a second project, genomic studies using diverse species of the plant family Solanaceae examine the evolution of resistance multi-gene families across species with varying degrees of relatedness.

Questions being addressed by both projects include the role of recombination in generating resistance gene diversity, comparative resistance gene diversity and genomic organization among closely related species, identification of quantitative trait loci (QTLs) that may be involved in plant resistance to a pathogen, and phylogenetic relationships among smut lineages. Answers to these questions are important in applied research looking for resistance gene function in plant breeding as well as for decision-making processes in agricultural practices to combat pathogens. The data are deoxyribonucleic acid (DNA) sequence and QTL mapping data that are analyzed using a variety of computer software. Data mining is also performed to add comparative data or additional markers to datasets the researchers generate in the laboratory. Other data include genetic markers for mapping and individual identification in population genetic studies. Bioinformatics tools are being developed to allow sorting through diverse gene sequences to identify those of potential value to agricultural plant disease resistance. Dataset sizes are on the order of 100s to 1,000s of sequences per organism with populations of 10–1,000 organisms. The analyses are computer-intensive both because of the dataset sizes, especially in terms of numbers of individuals or genomes being compared, and because permutation and data resampling are typical methods of generating statistical significance. The computational resources of the Computational Genetics Laboratory are enabling these researchers to analyze these large datasets.

Research Group

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Russell Spangler, Research Associate
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Joseph P. McFadden, Principal Investigator

Modeling the Effects of Land Cover Heterogeneity on Regional Climate and Hydrology in the Arctic

The arctic region provides a unique opportunity for modeling land-atmosphere interactions because its surface is characterized by a mosaic of a small number of vegetation types. This project uses a version of the Regional Atmospheric Modeling System (RAMS) that was developed for seasonal to interannual simulations (ClimRAMS) to study the effects of land cover heterogeneity on the climate and hydrology of arctic Alaska. The model represents the effects of vegetation, seasonal permafrost evolution, snow accumulation, and snowmelt, and the resulting changes in surface moisture and energy exchange. The Scientific Development and Visualization Laboratory is being used to develop a coupled modeling system that will incorporate a snow-transport model (Snow-Tran-3D) and a new, community land surface model (CLM).

Simulations can now be performed for 12- to 13-month periods using three two-way interactive, nested model grids. The model grids have horizontal resolutions of 60, 20, and five kilometers. The next phase of the research is to increase the horizontal resolution by a factor of four or five, increase the time period being simulated, and implement ensemble or factorial model experiments. This research has focused on an arctic domain; however, the modeling approaches developed are valuable for other regions characterized by a high degree of land cover heterogeneity.

Robert W. Sterner, Principal Investigator

Mechanistic Analysis of Biomanipulation in Shallow Lakes

Reduced water transparency, macrophyte abundance, and invertebrate abundance in turbid-state wetlands decrease the value of these ecosystems as habitat for wetland-dependent organisms such as waterfowl and amphibians. Thus, state and federal agencies managing wetlands of Waterfowl Production Areas and Wildlife Management Areas are interested in developing techniques that shift wetlands from turbid to clear-water states by reducing the abundance of undesirable fish. One of the most promising techniques is biomanipulation, or stocking of piscivorous (fish-eating) fish in turbid-state wetlands. However, the ability of biomanipulation to shift these wetlands to a clear state and the ecological mechanisms responsible for success and failure are poorly known.

These researchers are assessing the success of biomanipulation in shifting turbid-state prairie wetlands to a clear state, and will also elucidate mechanisms responsible for both success and failure. To meet these objectives, they are studying 20 shallow lakes in western Minnesota. They have biomanipulated 10 of these lakes, with the other 10 serving as controls. This study involves extensive collection of repeated measures data on numerous response variables over multiple years. Because of the large amount of data involved, the researchers are using the Computational Genetics Laboratory for this project.

Research Group
Kyle Zimmer, Research Associate

Susan I. Gibson, Principal Investigator

Identification of Sugar-Regulated Genes From the Model Plant *Arabidopsis thaliana*

The levels of soluble sugars, such as glucose and sucrose, are known or postulated to help regulate diverse aspects of plant development, metabolism, and physiology. Although the role of sugar levels in some plant processes has been well documented, whether sugar levels help regulate many other processes remains unknown. In addition, very little is known about the molecular mechanisms by which plants sense and respond to sugar levels. To help address these questions, these researchers are using Affymetrix GeneChips containing information from ~24,000 *Arabidopsis* genes to identify those plant genes that are regulated by sucrose, glucose, mannose, and/or sorbitol at the steady-state messenger ribonucleic acid (mRNA) level. They are using the resources of the Computational Genetics Laboratory to analyze this data to determine which genes are expressed at significantly different levels in response to feeding with different sugars.

Research Group

Yadong Huang, Graduate Student Researcher
Donna Pattison, Graduate Student Researcher

Ian M. Armitage, Principal Investigator

Structure/Function of Biomolecules Involved in Immune Suppression and Cellular Metal Homeostasis

These researchers are using biomolecular nuclear magnetic resonance (NMR) methods to forge new inroads into:

- The structure and metal exchange properties of proteins involved in the maintenance of metal homeostasis *in vivo.*
- Structural/functional studies of select molecules involved in the immune response.
- The structure, dynamics, and mechanism of activation of specific zinc finger deoxyribonucleic acid transcription factors upon zinc binding.

The researchers use the Basic Sciences Computing Laboratory to process multidimensional NMR sets, to calculate three-dimensional biomolecular structures, and to visualize those calculated structures.

Research Group and Collaborator

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Leonard J. Banaszak, Associate Fellow

Structure/Function Studies of Biological Macromolecules

This group's research involves biochemistry, molecular biology, and x-ray crystallography for structure determination and functional characterization of proteins. They are continuing to perform structural studies on adipocyte lipid binding protein (ALBP), liver fatty acid binding protein (LFABP), lipovitellin, and microsomal triglyceride transfer protein (MTP). Other projects include the enzymes malate dehydrogenase, isocitrate dehydrogenase, short chain L-3-hydroxyacyl CoA dehydrogenase, and phosphoglycerate dehydrogenase. A new project has been started as well, the structural determination of the photosystem II protein complex. The projects can be grouped into three categories:

- Lipoproteins and lipid-protein interactions.
- Protein import.
- Enzyme structure and mechanisms.

In the first category, the group is attempting to solve the crystal structure of microsomal MTP. MTP is a heterodimeric polypeptide involved in transport of neutral lipids and phospholipids between membranes. It is required for the assembly of plasma very low-density lipoproteins in the liver and chylomicrons in the intestine. The smaller subunit of MTP has been identified as protein disulfide isomerase. Pure MTP in complex with protein disulfide isomerase is now available from recombinant human carrier deoxyribonucleic acid (cDNA) expression, but crystals of this complex are difficult to obtain. The group is working on improving the quality of the phase data so that a more interpretable electron density map can be created for MTP purified previously from bovine liver. Other work is directed at expression, purification, and crystallization of fragments of human MTP.

In the category of protein import, one project involves precursor sequence structure comparisons. The transit of proteins into intracellular organelles requires amino terminal precursor sequences that are cleaved on import to form mature protein. These amino terminal precursor sequences determine the target organelle for protein import, but there is little information about their structures. A prior structure of the precursor form of watermelon glyoxysomal malate dehydrogenase showed a disordered amino terminal but otherwise resembled the mature protein. Therefore, the project has grown to encompass studies on the precursor-proteins named yeast mitochondrial fumarase, yeast malate dehydrogenase, and yeast mitochondrial isocitrate dehydrogenase. The group has crystals and preliminary data for both the precursor and mature forms of the isocitrate dehydrogenase. They are performing crystallization trials for the fumarase and the malate dehydrogenase.

In the final category, the group is performing structural studies of the photosystem II protein complex. An atomic resolution structure of this protein complex will help elucidate how light energy can be coupled to the generation of chemical energy. The group has succeeded in purifying active photosystem II complex and has begun crystallization trials.

Research Group and Collaborators

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James R. Thompson, Faculty Collaborator
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Bridgette A. Barry, Principal Investigator
Darrin M. York, Co-Principal Investigator

Density Functional Calculations on Tyrosyl and Chlorophyll Radicals

In plant photosynthesis, reaction centers convert light energy into a stable charge separation. Tyrosyl radicals and chlorophyll cation radicals are intermediates in these electronic transfer reactions in photosynthetic reaction centers. These researchers are performing density functional calculations to determine the electronic structure of neutral tyrosyl radicals and chlorophyll cation radicals in the gas phase in the presence and absence of key hydrogen-bonding interactions. Spectroscopic properties of experimental interest, such as vibrational frequencies, isotope shifts, and hyperfine coupling constants, are derived during this process. In order to gain insight into the structure of these species in photosynthetic proteins, the researchers compare the results with experimental data acquired from photosynthetic reaction centers and from model compounds in solution. These calculations will set the stage for future work exploring the nature of electron transfer intermediates using a hybrid quantum mechanical/molecular mechanical approach.

Research Group
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Colette Sacksteder, Research Associate
Bengt Svensson, Research Associate

Victor A. Bloomfield, Principal Investigator

Metal Binding to Nucleic Acids

Divalent cations, particularly magnesium, strongly influence the structure and biochemical activity of nucleic acids. Although many aspects of magnesium binding to nucleic acids have been studied in detail, questions still remain concerning the binding modes. Both nucleic acids and cations are strongly hydrated and their interaction is accompanied by release of water molecules from their hydration shells. Due to this fact, the binding modes are distinguishable by hydration measurements. The hydration approach is especially valuable because of the difficulty of studying Mg^{2+} in solution by other techniques. It does not possess paramagnetic properties and heats of binding to nucleic acids are usually small, although free energy of binding is considerable, which reveals the entropic nature of the binding. The increase in entropy usually is attributed to dehydration.

Volume and compressibility effects of Mg^{2+} binding to poly(rA) correspond to inner-sphere complex with three–four direct contacts, while almost no hydration effects have been seen arising in binding to its deoxy analog, poly(dA), indicating a mostly delocalized binding mode. In addition, optical and calorimetric investigations revealed no influence of Mg^{2+} on poly(dA) properties, while it stabilizes and readily aggregates poly(rA) single-helices. Molecular modeling reveals that binding of Mg^{2+} to adjacent phosphates and N7 of adenines in poly(rA) is sterically possible, while the backbone conformation of poly(dA) with C2′-*endo* sugar puckering is not favorable for site binding: interphosphate distances are longer, and C2′ of ribose is situated between adjacent phosphates, making Mg^{2+} binding sterically impossible.

Research Group
Besik Kankia, Research Associate

Bianca M. Conti-Fine, Principal Investigator

Modeling the Folding of Human T Cell Receptors That Recognize Unrelated Sequences

The ability to recognize unrelated sequences is not uncommon among T cell receptors (TCRs). It may even be an intrinsic characteristic of all TCRs. The TCR's ability to cross-react with different targets may be important for increasing the T cell repertoire. Also, it is possible that autoimmune phenomena are triggered by T cells activated by exogenous antigens and able to cross-react with epitopes from self-antigens.

In the lab, these researchers have propagated monoclonal $CD4^+$ T cell lines from healthy subjects that are able to recognize the same unrelated sequences. Each T cell clone expresses a different TCR, as judged by the sequence of their Vα and Vβ regions. The researchers have now identified the sequence for the Vα and Vβ regions of several such cross-reactive TCRs.

The goal of this project is to take advantage of the coordinates of the many solved TCR structures to model the sequences the researchers have obtained. This will allow identification of characteristics that would explain their cross-reactivity with unrelated sequences.

This group has begun a new project to identify $CD4^+$ T cell epitopes on coagulation factor VIII (fVIII). The development of antibodies that neutralize fVIII's procoagulant function is a serious complication that affects approximately 25% of people with severe hemophilia A. The synthesis of fVIII inhibitors requires the activation of fVIII specific $CD4^+$ T cells, so immunologic tolerance of those $CD4^+$ T cells should be an effective mechanism to prevent the development of fVIII inhibitors. Identification of the sequence regions of fVIII that are recognized by fVIII-specific $CD4^+$ T cells is crucial for the development of fVIII specific tolerization procedures. The researchers are using models of the crystal structure of fVIII to investigate the structural characteristics of peptide sequences recognized by fVIII specific $CD4^+$ T cells, to determine if they have structural features typical of immunodominant universal $CD4^+$ epitopes identified on other protein antigens.

Research Group and Collaborator

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Mark Reding, Faculty Collaborator
Yexun Wang, Graduate Student Researcher

John D. Lipscomb, Principal Investigator

Structure and Mechanism of Oxygenase Enzymes

Oxygenase enzymes use molecular oxygen to oxidize a wide range of biological and manmade compounds with the incorporation of one or both atoms of oxygen from molecular oxygen in the products. These researchers are using supercomputing resources for two studies in this area.

The first project studies 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 O_2. 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. In collaboration with Douglas H. Ohlendorf's group, these researchers have solved the crystal structures of three of these enzymes. The supercomputers are being used to examine the crystal structures and to plan site-directed mutagenesis studies.

The second project studies another type of oxygenase that is typified by methane monoxygenase. 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 monoxygenase. Again in collaboration with the Ohlendorf group, these researchers have solved the crystal structure of the critical hydroxylase component and are using the supercomputers to visualize the structure and to plan mutagenesis studies.

Research Group and Collaborator

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Codrina Popescu, Research Associate
Michael Valley, Graduate Student Researcher
Matt Wolfe, Graduate Student Researcher

David H. Live, Principal Investigator

Structure and Dynamics of Mucin Glycoprotein Motifs

These researchers are using the computational and visualization resources of the Supercomputing Institute for an ongoing project to determine the structural and dynamic properties of mucin motifs. These motifs, characterized by regions of highly O-glycosylated protein, can be found in secreted mucin glycoproteins, in mucin domains of integral membrane cell-surface glycoproteins, and as components of the glycoprotein complexes in connective tissue. They can function both as purely structural elements, and in molecular recognition by virtue of their ability to display a variety of carbohydrate epitopes on the same protein core. These researchers have recently reported on the structure of a mucin glycopeptide that has offered new insights into the intramolecular interactions between sugar and peptide components that aid in understanding the conformational features displayed by mucins. A noteworthy aspect of the nuclear magnetic resonance (NMR) experiments was strong evidence for a well-defined organization even for a short mucin segment based on a glycosylated pentapeptide STTAV from the cell surface protein CD43. The importance of the comparatively rigid conformation in the physical properties related to mucin solutions, and in their ability to display locally high concentrations of carbohydrate epitopes in enhancing interactions with receptors, has prompted a more extensive investigation of the dynamic properties of such structures. Using the reported structure as a basis, the researchers are now carrying out and analyzing ^{13}C NMR relaxation measurements and molecular dynamics calculations to further understand the properties of mucins.

Collaborator

Ajay K. Royyuru, IBM Computational Biology Center, T. J. Watson Research Center, Yorktown Heights, New York

Hiroshi Matsuo, Principal Investigator

Structural Study of Nonsense Mediated mRNA Decay

One-third of all known gene mutations associated with diseases result in premature stop codons (PSCs) in their messenger ribonucleic acid (mRNA). These PSC mutant mRNAs would produce truncated deleterious proteins if translated. Whether RNA is degraded via the nonsense mediated decay (NMD) pathway is determined by translation events. During translation, the ribosome removes proteins attached to mRNA, including proteins that would otherwise trigger NMD. In the case of the PSC mutant mRNA, the ribosome halts at the premature stop codon and fails to remove proteins attached to the remaining mRNA sequence. One such protein complex, named "exon-exon junction complex (EJC)," binds all spliced mRNAs at 20–24 nucleotides upstream of splice sites. This complex includes RNA binding proteins that anchor the complex to mRNA and interact with proteins require for NMD.

This group's goal is to determine the structures of these proteins involved in the EJC by using nuclear magnetic spectroscopy (NMR). Since NMR is a powerful method of studying protein-protein interaction, this should provide fundamental knowledge of the structure of EJC and how EJC triggers the NMD. Supercomputing resources are necessary because of the large size of the NMR datasets: calculation of a protein-protein complex involves 6,000 atoms in molecular dynamics.

Research Group

Matthew Devany, Graduate Student Researcher
Prasad Kotharu, Graduate Student Researcher

Kevin H. Mayo, Principal Investigator

Structure and Dynamics of Proteins and Peptides

This research group uses the resources of the Basic Sciences Computing Laboratory to investigate the structure and dynamics of proteins and peptides by using nuclear magnetic resonance (NMR) spectroscopy. After deriving inter-nuclear distance and angular constraints from various NMR experiments, the researchers use computer modeling to derive the best set of structures to the experimental data. The structure is derived with simulated annealing and molecular dynamics calculations, and relaxation matrix calculations are used during structural refinement.

In related research, the group is studying the internal motions in proteins and peptides. They use molecular dynamics simulations 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.

A new project using the supercomputers involves native human platelet factor 4 (PF4), an asymmetric homotetrameric protein (seventy residues) known for its anticoagulant heparin binding activity. A chimeric mutant of PF4 called PF4-M2, which substitutes the first 11 N-terminal residues for the first eight residues from homologous interleukin-8 (IL8), forms symmetric

Kevin H. Mayo, Principal Investigator

homotetramers with essentially the same heparin binding activity as native PF4. Recent experiments by this group revealed that IL8 interacts with PF4 and PF4-M2. The researchers are using molecular dynamics simulations of IL8-PF4 and IL8-PF4-M2 heterodimers to find out their stability.

Research Group

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Douglas H. Ohlendorf, Fellow

Structural Analysis of Macromolecules

The work in the Ohlendorf laboratory involves creating and refining structural models of macromolecules using diffraction data, geometric constraints, and/or structures of homologous molecules. The goal of this research is to produce models that are sufficiently accurate 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.

The structural analysis of macromolecules was carried out in order to understand the structural basis of how macromolecules function. The current focus is on two groups of proteins—dioxygenases that use metal ions to cleave aromatic rings and gram-positive virulence factors. The researchers used the resources of the Supercomputing Institute to refine structures of substrate and inhibitor complexes of mutants of protocatechuate 3,4-dioxygenase (PCD), homoprotocatechuate 2,3-dioxygenase (HPCD), and 1,2-catechol dioxygenase (CTD), and to solve and refine the structures of several putative virulence factors from gram positive pathogens.

Work on the PCD system involves PCDs from three organisms—*Pseudomonas 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. The reaction is interesting because cleavage of a stable aromatic ring occurs without the use of exotic cofactors. In PCD the cleavage is between the vicinal hydroxyls (intradiol) and is accompanied by a non-heme Fe^{+3} ion.

As with PCD, in HPCD a single metal ion is used to cleave an aromatic ring. Unlike PCD, this

Continued on next page

Douglas H. Ohlendorf, Fellow

cleavage is adjacent to the vicinal hydroxyls (extradiol) and utilizes a non-heme Fe^{+2} ion or an Mn^{+2} ion. Work on this protein is focused on metal specificity as well as substrate selectivity. The group has refined the structures of HPCD from two organisms in five space groups.

Like PCD, CTD is an intradiol dioxygenase incorporating both atoms of molecular oxygen into an organic substrate using a non-heme ferric ion. But where the PCDs being studied contain six or more protomers each containing two polypeptide chains, CTD is a dimer of a single polypeptide chain. In addition, the substrate specificity is different in that CTD does not tolerate a carboxylate group on the aromatic ring para and meta to the hydroxyls. It is possible to select for mutants of CTD that have extradiol activity. The group is refining crystals of a chlorocatechol 1,2-dioxygenase (C1CTD), and they are studying two mutants of CTD.

Superantigens are operationally defined by a serotype-specific of $CD4^+$ T-cells. Typically only 0.0001–0.01% of helper $CD4^+$ T-cells respond when presented with an antigen. But when exposed to a superantigen such as toxic shock syndrome toxin-1 (TSST-1), as many of 20% of these helper T-cells respond by releasing large amounts of cytokines, producing fever, vomiting, diarrhea, shock, and sometime death. Analysis of recently completed sequences of *Staphylococcus areus* and *Streptococcus pyogenes* strains has revealed over three dozen open reading frames (ORFs) encoding putative pyrogenic toxin superantigens (PTSAgs). Preliminary data show that these ORFs are expressed in nature. The group is studying these molecules through structural and biological analyses. They are cloning, expressing, and crystallizing a number of putative new PTSAgs revealed by the genomic sequences of strains of *S. areus.*

Exfoliative toxins A (ETA) and B (ETB) from *S. aureus* are the causative agents in staphylococcal scalded skin syndrome. Although they are superantigens, there is no structural homology with other superantigens. In addition, their exfoliative activities depend upon a putative proteolytic activity. The group has defined the structures of several ETA mutants.

Enterococcus faecalis is a frequent cause of urinary tract infections and of endocarditis. In addition, *E. faecalis* is receiving attention because of its ability to generate and spread antibiotic resistance. Conjugation is an important mechanism for the spread of genetic information. Aggregation substance (AS) is involved in bringing bacteria into physical contact. The product of the *prgX* gene encodes for a receptor of the expression of conjugation proteins (e.g., AS), subject to the presence or absence of a seven amino acid pheromone. The group has grown crystals of *prgX* that diffract to high resolution, and they have collected an initial diffraction data set.

Research Group

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Greg Vath, Graduate Student Researcher
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David D. Thomas, Fellow

Muscle Biomolecular Dynamics

The goal of this group's research is to understand the molecular dynamics of force generation and movement in muscle. The orientation and mobility of contractile proteins can be deduced by examining and deconvoluting the electron paramagnetic resonance (EPR) spectra and anisotropy decays of spin labels and optical probes attached to the particular components, and can test models of molecular motion by simulating the EPR spectra and anisotropy decays predicted by the models. Specifically, molecular dynamics simulation can produce a trajectory of an attached probe from which EPR spectra can be directly simulated. In this way, the researchers can design effective site-specific probes and test models of muscle protein dynamics.

Research Group and Collaborators

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Kylie J. Walters, Principal Investigator

Using Nuclear Magnetic Resonance Spectroscopy to Reveal Protein Structures and Protein–Protein Interactions

These researchers are using nuclear magnetic resonance (NMR) spectroscopy to reveal protein structures and protein-protein interactions. Projects in the laboratory focus on proteins associated with human cancers, with the goal of using structural knowledge to design molecular inhibitors against specific oncoproteins. One major area of interest is the study of proteins associated with acute myeloid leukemia (AML). AML is associated with fusion proteins, produced as a result of chromosome translocations. Often the fusion proteins involve dimerization domains of one protein fused to a protein tyrosine kinase. Such tyrosine kinase dimers are constitutively active and misfunction to cause cancer. The researchers are using their structural knowledge of the dimerization domain of a fusion protein associated with AML to design a molecular inhibitor that blocks dimerization.

Research Group

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Alan Lueke, Graduate Student Researcher
Qinghua Wang, Graduate Student Researcher

These researchers are also studying the mechanisms that have evolved in mammals for deoxyribonucleic acid (DNA) repair. Nucleotide excision repair (NER) and base excision repair (BER) remove damaged DNA, which could otherwise cause cell death, tissue degeneration, aging, and cancer. The hHR23 proteins are required for recognition of damaged DNA and stimulation of NER, which they mediate by interacting with the xeroderma pigmentosum group C protein. With a similar function in BER, the importance of these proteins is further evidenced by the embryonic lethality in mice that results from their deletion. The hHR23 proteins also play a role in proteasome-mediated degradation, suggesting that they serve as a link between regulated protein degradation and DNA repair, two processes crucial for proper cellular function. Using the resources of the Basic Sciences Computing Laboratory, these researchers are solving the solution structure of the 40 kDA hHR23a protein. Furthermore, by using NMR spectroscopy, they are elucidating the proteasome-binding surface of hHR23a. From this knowledge, they will design mutant versions of hHR23a that no longer bind the proteasome. These mutant versions will be used in *in vivo* assays to ascertain the relevance of the hHR23-proteasome interaction in NER.

Carrie M. Wilmot, Principal Investigator

X-ray Crystallographic Studies of Reaction Intermediates in Proteins Containing Organic or Metal Co-Factors

This research focuses on the dynamics of molecular catalysis, particularly involving novel co-factors and metal ions, and the role played by metalloproteins in disease states. The principal tool of the research is macromolecular x-ray crystallography. The project involves freeze trapping catalytic intermediates in the crystal, both anaerobically and aerobically, leading to "snapshots" along the reaction pathways. These can be assembled into "movies of catalysis" at the molecular level. By understanding these reactions in such detail, better drugs can be designed, proteins can be rationally engineered for biotechnological purposes, and chemists can design simpler industrial catalysts to control analogous reactions. Specific topics of interest to this group include structural enzymology involving the co-factor tryptophan tryptophylquinone of methylamine dehydrogenase, structural enzymology of the dinuclear copper-containing enzyme tyrosinase, and the role of copper redox chemistry in the progression of Alzheimer's disease.

The researcher are using the Basic Sciences Computing Laboratory to solve the phase problem and to visualize, build, and refine models against the x-ray crystallographic data. They are also producing images for presentations and publications and are using various bioinformatics tools to mine the genomics databases for related proteins.

Research Group and Collaborator

Brian Brazeau, Research Associate
Ed Hoeffner, Staff
Arwen Pearson, Research Associate
Atsuko Satoh, Graduate School of Science, Osaka City University, Osaka, Japan
Kevin Watts, Graduate Student Researcher

Judith G. Berman, Principal Investigator

Candida Albicans Genome Database for Use With Microarray Analysis

Candida albicans is an important fungal pathogen of humans that is especially prevalent in immunosuppressed patients such as those infected with HIV (human immunodeficiency virus). The *C. albicans* genome has been sequenced. These researchers are generating a database of information about *C. albicans* genes that will provide context to microarray data.

These researchers are part of a consortium of investigators. Work being performed at the University of Minnesota has begun with identification of the full set of open reading frames (ORFs) present in the currently available *C. albicans* sequence. As part of this, these researchers are establishing a database to keep track of each ORF and to eventually link them with the standardized ORF names that will be made public by the sequencing group at Stanford University. In addition, the researchers will use the sequence data to design primer pairs to be synthesized for each ORF. The primer pairs will be synthesized at the University of Illinois, and then sent to the University of Minnesota for amplification.

Research Group

Eric Benson, Research Associate
Theodore Lindsay, Research Associate

Robert J. Brooker, Principal Investigator

Membrane Transport Proteins

These researchers are studying the structure and function of membrane transport proteins, which are important in a variety of cellular processes. They are using the facilities in the Basic Sciences Computing Laboratory, including genomic software and crystal structure and modeling programs.

Research Group

Samanda Durand, Undergraduate Student Researcher
Heather Hrondey, Graduate Student Researcher
Jerry Johnson, Research Associate
Liz Matzke, Research Associate
Jinyan Zhang, Research Associate

Duncan J. Clarke, Principal Investigator

Analysis of Yeast Cell Cycle Control

In this new project, the researchers are trying to understand mechanisms that cause genome instability. In humans, genome instability contributes to the incidence of birth defects and spontaneous abortion and is a key factor in the etiology of cancer. In more specific terms, these researchers are working on cell cycle checkpoint controls, sister chromatid cohesion, chromosome dynamics, and ubiquitin-dependent proteolysis. Each of these related areas is critical for the maintenance of a stable genome. This project uses yeast as a model system to rapidly discover new concepts that can then be translated to the human system. Yeast genetics and cell biology are used to investigate basic aspects of eukaryotic cell cycle control that are relevant for cancer research. Budding yeast is used as a model organism, providing the most powerful genetic tools that are available to researchers today. The researchers are relying heavily on information contained in several databases, and are using the Basic Sciences Computing Laboratory for their work.

Research Group

Catherine Andrews, Research Associate

David A. Largaespada, Principal Investigator

Patterns of Plant Gene Family Evolution

This research group uses the EXPRESSIONIST software program at the Computational Genetics Laboratory to analyze Affymetrix microarray data. One of these projects compares the gene expression profile of acute myeloid leukemia (AML) cell lines with and without mutations in the NF1 gene, or with and without expression of the NF1 GAP-related domain. Another project compares the chemotherapy-resistant derivatives of several AML cell lines.

Research Group

Suzanne Grindle, Research Associate
Diane Hasz, Undergraduate Student Researcher
Kelly Morgan, Undergraduate Student Researcher
Kevin Roberg-Perez, Research Associate

Michele Boldrin, Principal Investigator

The Cost of the Business Cycle

This project investigates the cost of the business cycle in a heterogeneously educated household economy. The researchers first used data from the Panel Study of Income Dynamics and the Current Population Survey to investigate the effect of the business cycle over wage and unemployment durations of people with different income levels. Then, they used that data to calibrate a stochastic general equilibrium model and analyzed the welfare effects of the business cycle. The researchers used the facilities of the Supercomputing Institute to solve the associated Bellman equation, which contains a large number of state variables.

Collaborator

Juan Rubio-Ramirez, Federal Reserve Bank of Atlanta, Atlanta, Georgia

Varadarajan V. Chari, Principal Investigator

Solving and Estimating Dynamic General Equilibrium Models With Heterogeneity

These researchers study the properties of the Bayesian approach to estimation and comparison of dynamic equilibrium economies. They apply Bayesian statistics tools, which they developed in the past using Supercomputing Institute resources, to estimate and compare sticky price models widely used in the literature.

Research Group and Collaborator

Jesús Fernández-Villaverde, Department of Economics, University of Pennsylvania, Philadelphia, Pennsylvania

Juan Francisco Rubio-Ramirez, Graduate Student Researcher

Zvi Eckstein, Principal Investigator

Labor Mobility of Immigrants: Training, Experience, and Opportunities

The transition pattern of immigrants to a new labor market is characterized by high wage growth, a fast decrease in unemployment as immigrants find initial blue-collar jobs, and then a gradual movement to white-collar occupations. A central aspect of this process is the acquisition of local human capital in the form of the local language, on-the-job learning (experience), and participation in training programs provided by the government. This project focuses on the labor mobility and human capital accumulation of male immigrants who moved from the former Soviet Union to Israel and are characterized by their high levels of skills and education. The researchers have developed a dynamic choice model for employment and training in blue- and white-collar occupations, where the labor market opportunities are random and are affected by the immigrant's characteristics, his past choices, and his language knowledge.

The model fits the observed patterns of unemployment, employment by occupation, and training. The estimated rates of return to training are very high (13–19%) for most of the male immigrants. However, the estimated disutility from training and the 2% rate of return per quarter for local experience deter the immigrants from participation in training. The wage return to language knowledge is large, but imported skills have zero return in the new country. The researchers found that the effect of training on job offer probabilities has a larger impact on the immigrant's welfare than the wage return.

Research Group and Collaborator

Sarit Cohen, Department of Economics, Bar-Ilan University, Ramat-Gan, Israel

Suqin Ge, Research Associate

Zvi Eckstein, Principal Investigator
Michael P. Keane, Co-Principal Investigator

Estimation of Discrete Stochastic Dynamic Programming Models of Economic Behavior

The goal of this project is to develop new methods to solve and estimate discrete stochastic dynamic programming (DS-DP) models, and use these to study decision making in areas such as human capital investment, occupational choice, and investment in health. In recent years, it has become common in economics to model individuals who are making choices in dynamic environments as if they were solving a DS-DP problem to determine their optimal decisions. Empirical implementation of such models has been hampered because their solution and estimation requires that very high order numerical integrations be performed. These researchers are investigating the use of simulation methods to circumvent these integration problems.

The researchers are applying these methods to two problems. The first is an ongoing project on the effects of welfare policies on educational and occupational choices of young women. This is a major extension of the basic Keane-Wolpin model developed for young men, because it brings in fertility and marriage as additional decisions. When this model is completed, it will be useful for predicting a number of important questions about how public welfare policies aimed at women and children affect behavior. For example, the model can simulate how changes in these policies might affect teenage pregnancy rates, out-of-wedlock birth rates, and high school dropout rates. Preliminary results suggest that welfare benefits modestly increase high school dropout rates, while raising teenage pregnancy rates and only slightly raising out-of-wedlock birth rates.

The second project is a new study into the return-to-work decisions of previously employed women after they give birth. In the model, the women decide on a quarterly basis whether or not to return to work and whether to place the child in day care. The model can be used to assess the impact of day care and mother's employment on child outcomes such as early test scores.

Research Group

Abby Barker, Graduate Student Researcher
Ahmed Khwaja, Graduate Student Researcher
Eric Olson, Graduate Student Researcher

Gautam Gowrisankaran, Associate Fellow
Robert J. Town, Co-Principal Investigator

Bayesian Inference for Hospital Quality in a Selection Model

This project develops new economic methods to infer hospital quality in a model with discrete dependent variables and non-random selection. Mortality rates in patient discharge records are widely used to infer hospital quality. However, hospital admission is not random and some hospitals may attract patients with greater unobserved severity of illness than others. In this situation, the assumption of random admission leads to spurious inference about hospital quality. This study controls for hospital selection using a model in which distance between the patient's residence and alternative hospitals are key exogenous variables. Bayesian inference in this model is feasible but very computationally intensive using a Markov chain Monte Carlo posterior simulator. Results to date use data on 74,848 Medicare patients admitted to 114 hospitals in Los Angeles County from 1989 through 1992 with a diagnosis of pneumonia. They find the smallest and largest hospitals to be of high quality and public hospitals to be of low quality. There is strong evidence of dependence between the unobserved severity of illness and the assignment of patients to hospitals. Consequently, a conventional probit model leads to inference about quality markedly different than those in this study's selection model. The researchers are now analyzing preliminary results on heart bypass patients from throughout the state of California.

Shri Ramaswamy, Associate Fellow

Visualization and Characterization of Three-dimensional Bulk Structures of Porous Materials

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

This research attempts to visualize and characterize the three-dimensional bulk structure of paper and board using non-intrusive techniques. Recent work has explored the use of x-ray micro-computed tomography (x-ray CT) to visualize the structure of porous materials. This technique is far superior to other techniques and the researchers are able to view the entire three-dimensional structure of thick (~300 mm) samples. These images are being binarized (black and white) using methodologies developed by this group. The researchers then use the supercomputers to analyze the binarized images for pore structure characterization. Structural parameters of interest include pore size distribution, average pore diameter, porosity distribution and average porosity, tortuosity, available transfer surface area, and fiber-fiber bonded area.

Initial estimates of the structure characteristics indicate an immense potential for this approach. Recent work using x-ray microtomography on paper samples of varying structures indicates that the technique is capable of visualizing the structure. The researchers' methods to characterize the internal pore structures reveal interesting information on the anisotropic nature of the internal structure. Image analysis using high resolution x-ray CT images of different samples of paper indicate that the porosity, surface area, and tortuosity can be characterized reasonably well. Pore-size distribution of high resolution images are currently underway.

In addition, these researchers have developed a model to simulate the physics of simultaneous permeation and adsorption of liquid in porous media. The results indicate that, in addition to inherent absorption characteristics of cellulose fibers, the rate of permeation through the pore space has a strong influence on the overall absorption by porous media. The researchers are developing a nuclear magnetic resonance technique to visualize and characterize the transient three-dimensional structure of porous media during liquid penetration.

Research Group and Collaborators

Aron Cooper, Undergraduate Student Researcher
Amit Goel, Graduate Student Researcher
Manyank Gupta, Graduate Student Researcher
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Wei-Shou Hu, Faculty Collaborator
Shuyuan Huang, Research Associate
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Amod Modak, Graduate Student Researcher
Jesil Pujar, Graduate Student Researcher
Muhammad Ali Siddiqui, Graduate Student Researcher
Matt Ryan, Graduate Student Researcher

Patrick E. Hanna, Principal Investigator

Studies of Arylamine N-acetyltransferases

Arylamine N-acetyltransferases (NATs) are cytosolic enzymes that play important roles in the metabolism of drugs and other xenobiotics. The NATs catalyze the acetyl coenzyme A dependent acetylation of primary arylamine, hydrazine, and hydrazide functional groups. The NATs also catalyze the bioactivation of both carcinogenic arylhydroxylamines, through an O-acetylation reaction, and carcinogenic arylhydroxamic acids through an acetyl coenzyme A independent reaction. The overall objective of this project is to develop a comprehensive understanding of the molecular basis of the catalytic mechanism, the active site topologies, and the substrate specificities of mammalian NAT isozymes. The researchers have conducted three-dimensional homology modeling studies of hamster NATs based on the crystal structure of *Salmonella typhimurium* NAT. These investigations are being extended to include evaluation of the interactions of substrates and inactivators with NAT active sites. The results derived from these studies are expected to contribute to the design of isozyme-selective inhibitors of NATs.

Research Group

Zhijun Guo, Graduate Student Researcher
Gregory Vath, Research Associate
Haiqing Wang, Graduate Student Researcher

Rodney L. Johnson, Principal Investigator

Design and Synthesis of Blocker q Human T Cell KV1.3 Potassium

Blockers of potassium channel KV1.3 inhibit mitogen-induced activation of T cells. Therefore, potent and selective channel blockers could be used as immunosuppressive agents. Recently modeling studies have been conducted with scorpion toxins, which are known blockers of KV1.3 with inhibition on the pico- to nanomolar range. Based on this work, a model of KV1.3 has been established. Using this model as a reference, the researchers hope to develop potent and selective small molecule blockers of KV1.3.

Research Group

Abigail Fisher, Graduate Student Researcher
Ashish Vartak, Graduate Student Researcher

Philip S. Portoghese, Principal Investigator

Interaction of Opioid Ligands With Opioid Receptors

These researchers are building and evaluating dimeric opioid receptors according to theoretical scoring functions taken from protein homology and long time-scale molecular dynamics calculations. Bivalent ligands that have been found experimentally to bridge the opioid recognition sites in opioid receptor dimers are being used as "molecular rulers" to provide information on the distance between binding sites. This project uses the resources of the Basic Sciences Computing Laboratory and the Medicinal Chemistry/Supercomputing Institute Visualization–Workstation Laboratory.

A new, related project using the supercomputers involves building homology models of opioid receptors mu, delta, and kappa based on the x-ray structure of bovine rhodopsin. The researchers will build a phospholipid layer around the receptor models and create a molecular dynamics simulation. The purposes of this project are: to further optimize the structures of the opioid receptors, especially the amino side chains; to study the local conformational changes of the receptors when ligands are docked onto the recognition site; and to evaluate the possible interaction of extracellular loop II with the ligand as well as with other residues in the binding sites.

Research Group

Eyup Akgun, Research Associate
David J. Daniels, Graduate Student Researcher
Nicolette Fernandes, Research Associate
Rashmi Gupta, Research Associate
Dennis L. Larson, Research Associate
Sathit Niratisai, Graduate Student Researcher
Sarika Prabhu, Research Associate
Yan Zhang, Research Associate

David M. Ferguson, Fellow

Simulations of DNA Hairpin Loop Structures Using Molecular Dynamics

Deoxyribonucleic acid (DNA) hairpin loops are vulnerable spots on the DNA molecule and play an important role in the control of several important biological functions. Such DNA molecules are intermediates in cellular processes in which they are opened by enzymes—nucleases—to produce short single-stranded extensions. It has also been shown that this enzyme recognition is not entirely dependent on the sequence of the hairpin loop but may also be dependent on the structure of the hairpin loop.

Research Group and Collaborators

David J. Daniels, Graduate Student Researcher
John Goodell, Graduate Student Researcher
Brian Kane, Graduate Student Researcher
Gary Lam, Graduate Student Researcher
Quang Le, Department of Family Practice, Hennepin County Hospital, Minneapolis, Minnesota
Kenneth E. Lind, Graduate Student Researcher
Iain McFayden, Research Associate
Colleen Murray, Undergraduate Student Researcher
M. Germana Paterlini, Faculty Collaborator
Gennady Poda, Research Associate
Mahadevan Seetharaman, Graduate Student Researcher
Govindan Subramanian, Research Associate

Using molecular dynamics (MD) simulations, these researchers are addressing the question of whether the pattern of DNA hairpin opening by nucleases is dependent on the structural features of the hairpin loop. Observations from previous nuclear magnetic resonance (NMR) studies have shown that the palindromic duplex sequence 5′d(CGCGTATATACGCG)3′ is a dimer at lower temperatures and forms a hairpin loop structure at higher temperatures. The researchers are studying this hairpin loop structure using the AMBER code modules, and the structures obtained from the simulations will be analyzed in reference to the available NMR data. Based on the MD simulations, the researchers can correlate the structural features of the hairpin loop to the nuclease digestion pattern, which will provide new insights into the mechanism of DNA hairpin cleavage by nucleases.

Daniel M. Kroll, Principal Investigator

Mesoscale Simulations of the Statics and Dynamics of Complex Liquids

Particle-based simulation techniques have recently emerged as an attractive alternative to more traditional methods for studying phenomena as diverse as rarefied gas dynamics and the dynamics and rheology of "soft" materials such as polymer solutions and melts, biological macromolecules, colloids, and amphiphilic mixtures and membranes. There are several reasons for this. For example, phenomena involving rarefied gas dynamics and hypersonic flow often occur in regimes where the Knudsen number is not negligibly small, so that the continuum approximation breaks down and the Navier-Stokes equation is not valid. Similarly, complex fluids present a challenge for conventional simulation techniques due to the importance of thermal fluctuations and the presence of disparate time scales. The unique problems associated with the modeling and analysis of these systems has led to the development of new coarse-grained simulation techniques that mimic the behavior of atomistic systems on the length scales of interest.

This group's research involves the development and implementation of advanced simulation techniques for studying this class of problems. Specifically, the goals of this research are:

- To perform a detailed simulation study of the phase behavior and scattering intensity at bulk and film contrast in nonsymmetric microemulsion and sponge phases.
- To support the development and application of a new particle-based simulation technique for studying rarefied gas dynamics, flow and transport in complex geometries, and the dynamics and rheology of complex fluids.
- To study diffusion and transport in the brain's extracellular space.

Research Group and Collaborator

Thomas Ihle, Institut für Computeranwendungen, Universität Stuttgart, Stuttgart, Germany
Ravi Nandigam, Graduate Student Researcher
Erkan Tuzel, Graduate Student Researcher

Rory P. Remmel, Principal Investigator

Hepatotoxicity of Naltrexone

Naltrexone is an opiate antagonist that was approved in 1984 to help patients with a history of opioid dependence maintain an opioid-free state. During trials of naltrexone to determine its efficacy for the treatment of obesity and senile dementia, researchers observed an increase in the liver enzyme serum transaminase. These researchers are using the Medicinal Chemistry/Supercomputing Institute Visualization–Workstation Laboratory to investigate this interaction and synthesize analogues that will no longer be hepatoxic but will retain the potent antagonistic activity of naltrexone.

In addition, these researchers are trying to find bacterial enzymes with a high degree of homology to human glucuronsyltransferase, UGT2B7, which will eventually enable them to model the substrate requirements for the glucuronidation reaction to occur.

Research Group
Natarajan Kalyanaraman, Graduate Student Researcher

W. Thomas Shier, Principal Investigator

Transfection of Polyethyleneimine Derivatives

The use of polyethyleneimine (PEI) dendrimers as transfection vectors has shown promise over the use of traditional vectors such as viruses and liposomes. Their use as vectors has not been perfected to such a degree to be used *in vivo* for gene therapy. These researchers are investigating a design of alkyl derivatives of PEI with acid cleavable linkages that would release the transported deoxyribonucleic acid in the proper cell compartment. These derivatives take advantage of the high cationic density of PEI, and the endosomal uptake mechanism of eukaryotic cells. The researchers are using the Basic Sciences Computing Laboratory for this project.

Research Group
Terry Steele, Graduate Student Researcher

Natalia Tretyakova, Principal Investigator
David M. Ferguson, Fellow

Structural Studies of DNA Cross-Links

Deoxyribonucleic acid (DNA)-DNA cross-linking appears to be essential for the cytotoxic and anticancer activity of many anti-tumor drugs, including nitrogen mustards, nitrosoureas, and psoralens. The presence of a single interstrand cross-link can prevent DNA replication and transcription, eventually resulting in cell death and the inhibition of tumor growth. Paradoxically, DNA cross-linking is also a common mode of action of some potent carcinogens, e.g., 1,2,3,4-diepoxybutane (BET) and pyrrolizidine alkaloids.

Determining the reason for the difference in the biological outcomes of DNA cross-linking by bifunctional carcinogens and anti-tumor drugs is important for our understanding of the mechanisms of the action of these agents and for the development of anti-tumor agents with minimal side effects. Unfortunately, experimental studies of DNA cross-linking agents have been hindered by relatively low cross-linking yields and by the limitations of the current methodologies. In order to map the sites of cross-linking to specific DNA nucleobases, hot piperidine treatment is typically used to induce single strand breaks at the site of alkylation, followed by gel electrophoresis (PAGE). Although PAGE-based methods provide a sensitive way of visualizing drug attachment sites within DNA sequences, they do not find structural information and are limited to alkali-labile DNA modifications. For example, the potent carcinogen BET and the anti-tumor agent nitrogen mustard have been reported to have the same sequence preferences, linking the N7-guanine positions within 5′-GNC context. Abundant stable cross-links, presumably between adenine nucleobases, have also been detected, but could not be further analyzed by gel electrophoresis. The latter lesions were not observed following DNA treatment with the anti-tumor agent Mitomycin C. These researchers are further studying these potentially promutagenic lesions using molecular dynamics simulations of the cross-linked duplex DNA.

Research Group

Mahadevan Seetharaman, Graduate Student Researcher

Carston R. Wagner, Principal Investigator

Computational Analysis of Chemical-Induced Protein Dimerization

The control of protein-protein interactions is a necessary requirement for cellular biological processes. Synthetic systems that emulate this control, such as chemical inducers of protein dimerization (CIDs), have diverse potential as model systems, as bioprobes, and as therapeutic tools. These researchers have developed a CID system based upon bivalent methotrexate ligands (Bis-MTX) that dimerize dihydrofolate reductase (DHFR), and are investigating the role of ligand conformation in governing dimerization, the effects of protein surface cooperativity, and the contribution of individual residues to the dimer interface.

Experimental evidence from nuclear magnetic resonance, fluorescence, and size exclusion chromatography suggests that Bis-MTX adopts a surprisingly stable folded conformation in aqueous solution, $\Delta G(fold) = -4.1 \pm 0.3$ kcal/mole. The researchers are using modeling to guide their approach to defining this conformation, as well as an aid to the design of alternate ligands that explore these properties. Their investigations have also revealed surprising cooperativity between the surface of the dimerized DHFR in solution, in spite of known entropic barriers to such an interaction, $\Delta G = -3.4$ kcal/mole.

During this research period, the researchers performed dynamics simulations of the conformational behavior of a Bis-MTX ligand in explicit aqueous solvent. A series of nanosecond-length simulations suggested a set of possible folded solution conformations for this ligand. The researchers also studied the conformational behavior of chemically induced DHFR dimers in explicit aqueous solvent. Dynamics simulations are being used to investigate the effect of protein surface changes on dimerization-interface stability. Initial results suggest that the current simulation methods are capable of reproducing the observed stability of the chemically induced dimers.

Research Group

Jonathan Carlson, Graduate Student Researcher

David J. W. Grant, Principal Investigator

Utility of Molecular Modeling

The focus of this research is to develop and evaluate means of engineering the properties of drugs and excipients in solid state to improve the performance and quality of pharmaceutical dosage form. The researchers are studying the effects of different physico-chemical properties on the solid-state properties of drugs, both crystalline and amorphous.

The group is using molecular modeling to supplement and improve experimental results and inferences. Molecular modeling is also used to enhance the understanding of the physico-chemical interactions occurring in pharmaceutically important systems.

Research Group

Sharmistha Datta, Graduate Student Researcher
Yushi Feng, Graduate Student Researcher
Toshihito Hosokawa, Research Associate
Agan Sheth, Graduate Student Researcher
Justin Sjulson, Supercomputing Institute Undergraduate Intern
Deliang Zhou, Graduate Student Researcher

Ronald A. Siegel, Principal Investigator

Spatiotemporal Modeling of the Swelling of a pH-Sensitive Hydrogel

Research has shown that certain types of drugs, especially hormones, benefit from rhythmic and pulsatile delivery. For this reason, an implantable device for automatic, controlled drug delivery is desirable. Such a device would have a greater advantage if it used physiological substrates for its operation.

These researchers are studying a prototype device of this type. The device's operation is based on the properties of a pH-sensitive hydrogel (N-isopropyl acrylamide/methacrylic acid copolymer, or NIPA-co-MAA), which undergoes a first-order volume phase transition with thermodynamic hysteresis, with variation in pH. NIPA-co-MAA is used as a membrane to separate an enclosed chamber from the external environment. At high pH, the membrane is swollen and allows glucose to pass, while at low pH, the membrane is in the collapsed state and blocks glucose transport. The dynamics of pH in the oscillator chamber are driven by glucose flux into the chamber, which is governed by the glucose permeability of the membrane and enzymatic conversion of glucose to hydrogen ions. When the membrane is swollen the drug is released and glucose enters the chamber, driving the pH down; this causes the membrane to collapse and the glucose and drug permeability to drop. Glucose is then no longer supplied as a substrate for enzymatic conversion and the pH goes back up. Finally, the membrane re-swells and the cycle repeats. The results of these processes are oscillating values of intrachamber pH and permeability to glucose and drug. The researchers are using supercomputing resources to perform the mathematical modeling of this system. The goal of the modeling is to understand the effect of system conditions on the behavior of the hydrogel membrane in this highly non-linear system.

Research Group

Anish Dhanarajan, Research Associate
Jon Urban, Graduate Student Researcher

Mitchell Abrahamsen, Principal Investigator

Functional Gene Analysis of Bovine Gamma/Delta T-Lymphocytes in Response to Mucosal Pathogens

T-lymphocytes bearing the gamma/delta T cell receptor (TCR) are a subgroup of T cells whose function remains largely unknown. Evidence suggests that they are important in host responses against various pathogenic infections, but we have only limited knowledge of their biology. This project will use functional genomics techniques to analyze the entire repertoire of genes expressed in a specific cell population. Comparing gene expression profiles of gamma/delta T cells in response to various mucosal pathogens will allow these researchers to determine what gene products correlate well with and define the functional activities of gamma/delta T cells.

Research Group
Mingqi Deng, Research Associate

Alvin J. Beitz, Principal Investigator

Analysis of Mouse Spinal Cord mRNAs Using Affymetrix Microarrays

These researchers are using the resources of the Computational Genetics Laboratory to analyze gene expression data from Affymetrix microarrays. This project consists of two main areas, each of which is designed to measure changes in spinal cord messenger ribonucleic acids (mRNAs) in experimental animals compared to controls.

The first subproject focuses on alterations in spinal cord mRNA in a mouse model of multiple sclerosis (MS). It is known that myelinated axons in the spinal cord lose their myelin sheaths in patients with MS. The question remains as to what alterations occur in spinal cord mRNAs and proteins at various time points during the development of this demyelination process. The researchers are investigating changes in the mRNAs for cytokines, growth factors, and myelin proteins.

The second research area addresses the changes that occur in spinal cord mRNA in chronic cancer pain. The researchers have developed a mouse model of cancer pain and are analyzing the changes that occur in the spinal cord mRNA expression in these mice compared to naive animals.

Since cancer pain and MS are important clinical conditions, these two projects will not only advance knowledge of gene expression changes in the spinal cord in these disease states, but the data will be instrumental in developing novel approaches to treating these conditions.

Research Group
Mary Baddorf, Graduate Student Researcher
Jessica Lynch, Graduate Student Researcher

Sagarika Kanjilal, Principal Investigator
Vivek Kapur, Co-Principal Investigator

Comparative Cancer Genomics

This group's research is focused on elucidating basic mechanisms of cancer pathogenesis and progression using molecular and comparative genomic approaches. The project can be categorized into three thematic areas:

- Identification of molecular markers and gene-expression profiles in tumor development and progression.
- Characterization of the cancer genome through analyses of human and feline tumor carrier deoxyribonucleic acid (cDNA) libraries and cat bacterial artificial chromosome libraries.
- Elucidation of molecular response to chemotherapeutic agents and discovery of novel drug targets.

The group is using the resources of the Computational Genetics Laboratory to store and analyze batches of sequence files and microarray data sets, both from Affymetrix GeneChip and custom cDNA array experiments. Further work will involve visualizing, accessing, and querying the information using existing or custom software tools.

Research Group
Nilanjana Banerji, Research Associate

Vivek Kapur, Principal Investigator

Microbial Pathogenomics

The focus of this research program is to understand the basic processes by which bacteria cause disease and their hosts respond to infection. To address this problem, the researchers apply genomics tools, including whole genome sequencing, expression profiling using microarrays, and proteomics, to characterize microbial pathogens and the host response to infection.

Research Group
Lisa Herron, Graduate Student Researcher
Qing Zhang, Research Associate

Samuel K. Maheswaran, Principal Investigator

Molecular Characterization of the *Mannheimia Haemolytica* Leukotoxin Receptors

Pneumonic mannheimosis, caused by *Mannheimia haemolytica*, is the most common syndrome in the bovine respiratory disease (BRD) complex. In keeping with its primary status within the complex, the disease is the leading source of economic loss to the North American beef industry, and also significantly impacts dairy cattle health. The major virulence factor contributing to the pathology observed in the disease is the leukotoxin LktA. LktA is a member of the Repeats in Toxin (RTX) family of cytolysins and, besides possessing the major characteristics of the group, exhibits a unique specificity to ruminant leukocytes and platelets. Evidence suggests that much of the lung injury observed in the disease is caused by an inflammatory process in the lungs. The unique specificity of LktA to ruminant leukocytes has been reported to involve binding to the β2 integrin receptor CD18. CD18 is a common subunit of three β2 integrins: lymphocyte function associate antigen-1 (LFA-1, CD11a/CD18), Mac-1 (CD11b/CD18), and P15095 (CD11c/CD18). Subsequent work from this laboratory has suggested that LFA-1 exclusively is the receptor involved in the LktA binding.

Research Group

Dileepan Thamothatampillai, Graduate Student Researcher

Praveen Thumbikat, Graduate Student Researcher

The human homologue of bovine LFA-1 has been observed to interact with its natural ligand ICAM-1 using a defined domain in the CD11a subunit of the heterodimer. This defined domain named as the "inserted" (I) or "activation" (A) domain has been shown to be critical for ligand interactions. Preliminary work on cloning and sequencing of bovine CD11a from this laboratory has revealed that this domain is significantly conserved in the bovine homologue. Thus, the likelihood of this domain's involvement in LktA interactions with bovine LFA-1 is very high.

This project uses the resources of the Basic Sciences Computing Laboratory to model the bovine I domain based on its human homologue. This is helping the researchers to identify the key residues in the bovine LFA-1 ligand-binding region that are likely to mediate toxin binding. Furthermore, recent work on the human homologue has identified pharmacological inhibitors of LFA-1 binding which are directed at the I domain region. Therefore, the researchers are attempting to predict whether these structural inhibitors would perform a like function in the bovine I domain. The identification of an Lkt1-I domain interaction would aid greatly in designing more targeted drugs that may interfere with LktA-target cell interactions. These agents would prove useful adjuncts to antibiotics in disease therapy and prevent relapses necessitating multiple antibiotic usages.

Michael P. Murtaugh, Principal Investigator

Porcine Peyer's Patch Expressed Sequences Associated With Disease Resistance

Peyer's patches (PPs) are specialized immune tissues lining the small intestine of vertebrate species. Their anatomical location, their ability to sample microorganisms and molecules from the gut environment, and their organized lymphoid architecture have led to the hypothesis that PPs provide immune surveillance at enteric portals of pathogen entry, are both inductive and effector sites of immune resistance, and mediate oral tolerance to food antigens and commensal bacteria. Despite this critical role in host defense against enteric pathogens while preventing immune responses to food, detailed information about the biochemical and molecular mechanisms by which the PP executes its functions is lacking in all vertebrate species. Moreover, the absence of deoxyribonucleic acid (DNA) sequence information underlying PP biochemical functions interferes with the use of genetic selection to improve animal health and production. These researchers hypothesize that PP expresses genes with specialized functions to maintain mucosal immunity and resistance to enteric disease. To address this hypothesis, the researchers are cataloging the functional activities of the PP by identification of expressed sequences and localizing genomic regions involved in differential resistance to enteric disease by microsatellite linkage disequilibrium in a commercial swine resource population.

A PP molecular catalog, or transcriptome, will provide a foundation for long-term research programs to enhance the understanding of PP biology. Identification of genomic regions that segregate with enteric disease resistance will, with the help of comparative mammalian gene maps, result in the association of candidate PP expressed sequences with differential disease resistance. The findings will help to nominate PP expressed genes with roles in enteric disease resistance and further the development of genetic selection tools for livestock disease resistance.

Research Group

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Ioulia Ioffe, Principal Investigator

Term Structure of Interest Rates and Implied Market Friction: The MinMax Approach

It is often assumed that financial markets are frictionless. While serving well in some instances, in bond markets this assumption prevents researchers from obtaining an estimate of the term structure (TS) of interest rates. This is because bond markets are illiquid and bond prices are observed with errors. These errors are so large that they lead to violation of no-arbitrage conditions in the market. Researchers have had to settle for a second-best estimate of the TS (obtained via regression) at a cost of economically unrealistic assumptions of symmetric market frictions. The true shape of market frictions, however, is not known and generally is a highly complex issue. The methodology developed here avoids making detrimental assumptions. It facilitates empirical investigation of the shape of the market frictions and of the TSs that are simultaneously imputed from market data.

This methodology is based on no-arbitrage arguments and an assumption that in "efficient" markets, frictions will minimize maximum net arbitrage. The empirical investigation is performed in the Canadian and U.S. markets and involves implementation of non-linear optimization procedures. Preliminary results indicate that in both markets it is found that market frictions are not symmetric and the estimates of the TS produced via regression and the methodology developed here differ significantly. This difference is more pronounced in the Canadian market, which corresponds to the fact that the U.S. Treasury market is much more liquid than its Canadian counterpart.

William Li, Principal Investigator
Christopher J. Nachtsheim, Co-Principal Investigator

Model-Robust Designs, Non-isomorphic Orthogonal Designs, and Optimal Blocking Designs

The first object of this research is to construct model-robust designs that include supersaturated designs and response-surface design. Model-robust designs usually consider many different possible models that can increase exponentially with the run size. Thus, the problem is extremely computationally intensive. The second objective is to construct complete catalogs of non-isomorphic designs. Orthogonal designs are the most commonly used experimental designs in practice. The choice of optimal designs depends on two important things—criterion and complete catalogs of the candidate orthogonal designs.

These researchers are using a newly developed efficient algorithm and a theory based on the indicator function to construct complete sets of orthogonal designs with economic run sizes. The third objective, which is a follow-up to the second one, is to find optimal blocking schemes for commonly used orthogonal designs. Blocking is a commonly used technique to reduce unwanted variations in statistics. These researchers' recent results in complete catalogs of orthogonal designs can greatly facilitate the research in the optimal blocking designs.

Graham V. Candler, Fellow

Simulation of Reacting Flows

This group continued its research into two types of flows: high-temperature reacting flows and low-density flows. The overall goal of this work is to understand how finite-rate chemical reactions interact with fluid motion, and to determine how and when the Navier-Stokes equations fail in low-density applications.

This research has several technological applications. The researchers are using computational fluid dynamics (CFD) to study how very localized energy deposition (using a pulsed laser) can be used to control a supersonic flow. The researchers are now capable of simulating this complex process during all phases of laser energy addition, with very good agreement with experimental data during the initial formation of the resulting blast wave.

In related work, the researchers are modeling the generation of atmospheric pressure air plasmas. This will be used for applications to flow control and signature reduction and the study of very high-energy atmospheric re-entry flows for application to heat shield design for outer-planet sample return missions.

Other work by this group uses the CFD codes to study how and when the Navier-Stokes equations fail in high-speed supersonic flows and in low-speed micro-scale flows. The codes are used here based on the continuum conservation equations to compare with the direct-simulation Monte Carlo method. This approach models the flow using a kinetic theory based formulation that includes the motion and collisions of many millions of particles to obtain a statistically accurate flow field. This fundamental work will result in more accurate and efficient simulations of high-altitude flows and micro-scale flows for microelectrical mechanical system applications.

Another aspect of this research involves the advanced visualization of a new direct numerical simulation dataset of high Mach number reacting turbulent flows. The researchers are attempting to understand how turbulent motion is generated and sustains itself in high-speed boundary layers. This work is in itself new, but the datasets include the effects of finite-rate chemical reactions, so that the researchers can develop an understanding of how energy is transferred between the turbulent motion, the internal energy codes, and chemical energy codes. During this research period, they have developed a new model for shock-turbulence interactions. This work is the first of its kind, and will lead to greatly improved understanding of the physics of turbulent motion.

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Large Deformations in Nonlinear Elasticity and the Thermodynamics of Propagating Phase Boundaries

The goal of this program is to carry out a theoretical and computational investigation of coexistent phase structures in solids when subjected to external load, environment temperature, or electrical stimulation. The existence and growth of zones of evolving microstructure are not only responsible for the failure of materials, but also play an important part in the design of devices and in many emerging applications that depend on sophisticated nonlinear material behavior. As technology advances, it is clear that materials that support internal phase structures are becoming increasingly important, and a better understanding of the difficult mechanics and materials issues will surely enhance their applicability.

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 lead to highly localized large deformations. For solids, there are contemporary computational developments, iteration procedures, adaptive methods, and continuation techniques that are already being used successfully in the computation of regular boundary value problems that arise from nonlinear theories. Some of these ideas are also being used in this research, 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 kinetics require admissibility hypotheses, so-called "kinetic relations," to be solvable. These kinetic relations, while ensuring uniqueness, have questionable physical justification. These researchers are developing a thermomechanical model including capillarity, viscosity, and thermal conductivity. In this setting, the researchers hope to prove that the limiting solutions, as the capillarity, viscosity, and thermal conductivity approach zero, are the physically relevant ones. Because the free energy is nonconvex, the governing equations are of mixed type: hyperbolic in regions of pure single phase and elliptic in the intervening spinodal region. Continuing computations and analysis show that this is a promising method of calculating dynamic phase transitions. However, the researchers are also investigating other methods, including the determination of dependence on numerical methods. They are implementing and testing several finite difference and finite element methods for solving these equations and are developing their own approach. Part of the problem is to optimize the computations and to address the questions of parallelization and alternate numerical techniques.

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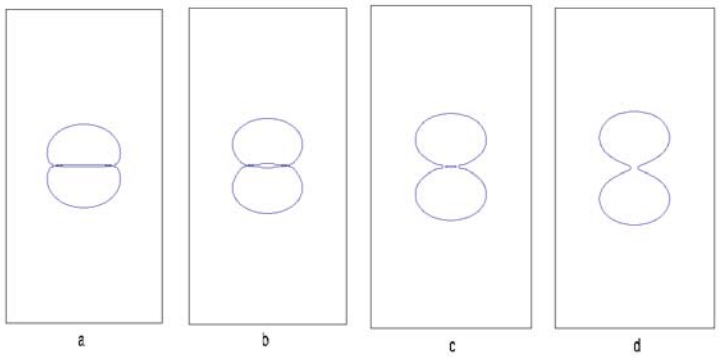
Ashley James, Principal Investigator

Numerical Simulations of Liquid Fluid Interface Flows With Topological Transitions

This research concerns the analysis of interfacial fluid flows and the development of concomitant computational methods, focusing on on topological changes, such as breakup and coalescence. These changes are important in numerous industrial, aerospace, biomedical, and environmental applications. In order to control such systems, one must have a detailed understanding of the fluid dynamics involved.

The James group has developed an interfacial flow solver to investigate the use of vertical vibration to cause droplet ejection. They are modifying the solver to improve its accuracy and extend its capabilities to analyze other physical systems. Most recently, the group has been developing a module to incorporate soluble surfactant. This capability will be used to determine the effect of soluble surfactant on the break-up of a bubble in an extensional flow. Tests of the original version of the module showed that the volume-of-fluid method used to capture the motion of the interface is a poor predictor of the surface area in a cell. Knowledge of this surface area is required to determine the local surfactant concentration. To remedy this problem, the researchers derived an additional equation governing the evolution of the surface area, and implemented its solution in the code. Tests of the new modules showed that the area is tracked accurately, and simulations of the bubble breakup problem have begun.

In another project, the interfacial flow solver code is being used to simulate the coalescence of two liquid drops. The researchers have performed simulations to determine the effect of the choice of boundary condition on the coalescence process. External forcing is applied as a hyperbolic flow, causing a drop to impact a symmetry line. Thus, the drop interacts with its mirror image. The boundary condition on the symmetry line can be chosen to prohibit coalescence, to make coalescence occur automatically, or to allow coalescence to occur selectively depending on local conditions.



Effect of van der Waals force on the symmetric coalescence of two drops. The strength of the van der Waals force is characterized by the dimensionless Hammaker constant, A. a) $A = 0$ (no van der Waals force). As the drops approach one another, a dimple forms between them, so coalescence occurs, at $t = 0.38$, at the rim of the dimple. b) $A = 1$. The process does not change qualitatively; although it is sped up by the van der Waals force, the drops do not flatten as much, and coalescence occurs earlier, at $t = 0.33$. c) $A = 10$. When the van der Waals force is increased, coalescence occurs even sooner, at $t = 0.29$, just after the dimple has begun to form, but before it has had time to grow radially. d) $A = 100$. For the largest van der Waals force considered, coalescence occurs at $t = 0.26$, before the dimple has time to form.

The response is quite different in the three cases. The researchers have also incorporated van der Waals forces into the momentum equations. Including van der Waals forces in the drop after coalescence, as well as in the gas film between the drops, had a significant impact on the response.

A new direction for this group is the study of the motion of an oil drop through a constriction, which is a model for porous media flow of petroleum during production from a deposit.

Research Group

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Daniel D. Joseph, Fellow

Direct Numerical Simulation and Modeling of Solid-Liquid Flows

This research group continued developing scalable, highly efficient parallel finite-element codes, called "particle movers," for the direct numerical simulation of the motion of solid particles in Newtonian and viscoelastic fluids, in both two and three dimensions. Development of two separate particle movers was the prime focus. One method to achieve this—the Arbitrary Lagrangian-Eulerian (ALE) particle mover—is a generalization of the standard Galerkin finite-element method that uses an unstructured mesh and the ALE scheme to handle the time-dependent domain. The second—the disordered local moment (DLM) particle mover—is a fictitious-domain method, in which the fluid flow equations are enforced inside, as well as outside, the particle boundaries. Both methods use a combined fluid-particle weak formulation in which the hydrodynamic forces and torques are eliminated.

The group is continuing with their efforts to improve the performance of the particle movers by tailoring the partitioning scheme to produce a division favorable to the multi-lever preconditioner they have used. They are also experimenting with a new narrow-band preconditioner based on a Schur complement formulation, which could greatly increase the efficiency of the iterative solver. Their matrix-free version of the ALE particle mover, based on an operator splitting method, will allow much larger problems to be solved. This code is being parallelized with the public software package PETSc. The parallel version of the three-dimensional DLM particle mover is also complete, and is being compared to results from the DLM code and the ALE code. They are also working on a parallel Poisson solver using the multi-level algorithm.

These codes are being used to investigate the fundamental dynamics of fluid-particle motions. The group is working to develop models of the lift force on particles in Newtonian and viscoelastic fluids. The researchers have also developed a method to simulate motions of general-shape particles. They attach two points, besides the center of mass, to each particle and move them according to the rigid-body motion of the particle in order to track this motion. The method was used to simulate ellipsoids settling in a narrow channel filled with a Newtonian fluid; the results agreed well with experimental results.

Research Group and Collaborators

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Computational Problems in Multicomponent/Multiphase Elastic Materials

These researchers are continuing their studies of microstructures formed in crystalline alloys. They are developing computational methods for studying microstructure in three dimensions, and are creating both diffuse and sharp interface models to study multicomponent diffusion and sequences of phase formation in thin alloy films.

In the first area, the researchers have developed and implemented a three-dimensional sharp interface model, which they have used to study the growth and coarsening of a single particle. Their next goal is to improve this method so it can account for the evolution of multiparticle systems.

In the second area, the researchers are improving their one-dimensional models to study diffusion and phase formation in layered systems. They are extending the models to two and three dimensions, and will use the two-dimensional model to study phase formation in multicomponent, multilayered thin films with solid-state reactions.

Research Group and Collaborator

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Krishnan Mahesh, Principal Investigator

Large-Eddy Simulation of Turbulent Flow in Complex Geometries

These researchers developed the computational capability to perform large-eddy simulation (LES) of turbulent flows in realistic engineering geometries. LES is a computational approach where one filters the unsteady Navier-Stokes equations, and numerically solves for the large-scales while modeling the effect of the smaller scales that have been filtered out. It is a solution approach that provides unsteady spatial data, in contrast to the popular Reynolds-averaged Navier-Stokes (RANS) equations. LES is, however, more computationally intensive. Also, LES has traditionally been restricted to simple geometries, such as channels, backsteps, mixing layers, and jets. The advent of massively parallel computers has allowed for the development of LES to a level at which it can be applied to engineering flows. In particular, predicting internal flows such as those found in gas-turbine combustors is a particularly appealing area, since the Reynolds numbers in internal flows are relatively low. Furthermore, the combustion process is dominated by mixing, which LES has been shown to predict considerably more accurately than RANS. Due to the broadband nature of turbulence, the numerical methods used to compute the RANS equations cannot be directly applied to simulate turbulence; in particular, the numerical schemes used for LES cannot be dissipative. Numerical dissipation competes with the dissipation that the LES model is trying to provide, so the LES model usually has no effect.

This research group has developed a non-dissipative, numerical algorithm for turbulent flow on unstructured grids. The use of unstructured grids allows arbitrarily complex geometries to be efficiently gridded. A novelty of the algorithm used is that it discretely conserves not only momentum, but also kinetic energy. This allows robustness without numerical dissipation. Such robustness is imperative to perform accurate simulations in complex geometries at high Reynolds numbers.

The primary goal of this research is to develop the capability to perform LES in configurations relevant to industry. Projects that the group is working on include simulation of turbulent jets in cross-flow, scalar mixing in turbulent jets, simulation of turbulent channel flow, simulation of propeller crashback, and study of flow around the saguaro cactus.

Research Group

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Cynthia A. Cattell, Associate Fellow

Kinetic Physics in the Earth's Magnetosphere

This research group is studying several aspects of the kinetic physics of planetary magnetospheres, including the excitation of waves in the Earth's auroral zone, wave particle interactions in the auroral zone and magnetotail, and particle energization in the magnetic field-reversed geometry of the magnetotail of the Earth. Fast Auroral Snapshot Explorer (FAST) satellite observations have provided the most detailed and complete measurements of the velocity space distribution functions of the plasma constituents in this region. FAST simultaneously collects data on electric and magnetic waveforms and has the capability to determine the propagation velocities. Recent work provided illumination on the relationship between cold and hot plasma modes. A new study examined wave modes excited by downflowing ions. Continuing investigation of FAST data focuses on:

- Modeling upward and downward ion flow and upward electron flow events.
- Improving the accuracy of the model distribution functions.
- Investigating the relationship of linear modes to nonlinear solitary waves.
- The relationship between electromagnetic and electrostatic modes.

This group is finishing studies of the effects of electromagnetic fields on particle trajectories, to determine whether the phase space structures observed when there are no perturbations are substantially modified. The electromagnetic fields occur on various spatial and temporal scales in the Earth's magnetotail. The group has completed the runs for studying the distribution functions and energization obtained when there are no waves for a number of different magnetic field models, including the T89, T87, and T96 Tsyganenko magnetic field models, to study what effects differing magnetic field models have on results for particle distributions and their moments. The work has shown that the choice of magnetic field model does have a large impact on the resulting particle distributions. The group is planning to make additional runs.

The researchers have also updated their previous studies of the impact of low-frequency waves upon energization and particle dynamics in the magnetotail to include the newer T96 magnetic field model. This work has shown that the presence of low-frequency waves in the magnetotail does have an impact on particle distribution, and therefore needs to be modeled accurately to gain a better understanding of magnetotail distributions, moments, and dynamics.

A new project based on this code examines motion of energetic particles in the electromagnetic fields of heliospheric shocks. This research will make use of data from the recently launched European Space Agency–National Aeronautics and Space Administration Cluster mission, which includes four satellites in a tetrahedral formation. The existence of any heliospheric shock (either bow-shock in the vicinity of a magnetized planet or a shock propagating in the interplanetary medium due to solar processes) requires a subtle population of particles that support it. The stability of a shock requires specific distribution of charged particles that form currents and charges that are self-consistent with the macroscopic magnetic fields

Continued on next page

Research Group and Collaborators

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and electric fields, respectively. Recent measurements from the Cluster satellites show detailed crossing across interplanetary shocks with a high resolution in electromagnetic fields. The group is investigating the motion of test particles in the observed fields in order to understand the formation of their charges and currents. They are particularly interested in the non-adiabatic behavior of electrons and their separation from the ions due to microscopic trajectories in the strong gradients of electric fields. The results of this work will shed light on realistic nonlinear structures and their stability in the presence of solar wind plasma, for a variety of solar wind parameters. The simulations require the use of supercomputing resources because of they include many thousands of particles and require gather-scatter facilities to get a significant phase space resolution.

Another project involves developing algorithms for analysis of datasets from multi-spacecraft missions. Building on work done by the scientists associated with the Cluster mission, this group is designing efficient analysis techniques that will be applicable to a wide range of satellite cluster configurations making *in situ* plasma and field measurements.

Thomas W. Jones, Fellow

Numerical Studies of Particles and Fluids in Astrophysics

These researchers continued their pioneering efforts 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. The researchers also apply this knowledge to the understanding of some recognized "key" astrophysical problems, especially the origins of the cosmic rays themselves and the nature of the most energetic phenomena in the universe—giant radio galaxies, supernova remnants, and enormous "cosmic structures" that form by gravitational collapse against the expansion of the universe.

Research Group and Collaborator

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Ian Tregillis, Research Associate

This work is based on state-of-the-art codes for compressible magnetohydrodynamics (MHD) and novel schemes for following the acceleration and propagation of cosmic rays, all developed by this group. This is an especially opportune time, since a new generation of x-ray and γ-ray astronomical observatories is coming on line. Several new satellites are offering the first high-quality x-ray and γ-ray data on radio galaxies, supernova remnants, and galaxy clusters to compare with theory. New ground-based high energy observatories will soon open entirely new windows on these phenomena. This group's efforts combined with the new experimental data represent the first time that genuine

Thomas W. Jones, Fellow

tests of the detailed physics have been possible.

One project during this research period used three-dimensional MHD simulations to study particle transport and radiation from radio galaxies. Radio galaxies are among the largest and most powerful accelerators of high-energy particles in the universe. They are also enormous repositories of energy, sometimes exceeding the total nuclear energy release of all the stars in the parent galaxy over the age of the universe. They represent the visible results of hypersonic plasma jets formed electromagnetically in the cores of otherwise ordinary galaxies. As the jets bore into the tenuous external media they generate rich shock complexes and fill huge cavities with relativistic, magnetized plasma. Those structures are known as radio galaxies to reflect that they are most easily seen through radio emission from the relativistic plasma. This phenomenon is now seen as a critical probe for a host of important astrophysical problems. This research group initiated the first computational study of the dynamics of radio galaxy flows that includes both the relativistic particles and the magnetic fields. They then initiated a "second generation" of simulations designed to follow the evolution of these objects longer than had been previously attempted by anyone. The researchers carried out three high-resolution simulations on a nonuniform 600 x 200 x 200 grid; these simulations also included time evolution of the momentum dependence of the relativistic electron distribution, so they are effectively four-dimensional.

This project is being extended to follow the interactions of radio galaxies as they interact with cluster media after the energy source of the radio galaxy has ceased. The researchers also have begun to study how these objects interact with cosmic cluster structures.

Another project of this group is three-dimensional, *N*-body/MHD simulations of cosmic cluster formation. One of the key discoveries of the 20th century was the highly homologous expansion of the universe. Within that expansion, however, are very evident local concentrations and even collapsed structures. Those concentrations result from initial density perturbations in the early universe that became gravitationally unstable and energetically bound. It is now possible to carry out very high-resolution simulations of this cosmological evolution. Using cosmological simulations, these researchers recently discovered the existence of extensive complexes of strong shocks. Other work by this group has shown the potential for these shocks to accelerate cosmic rays to high energies. These cosmic rays may even be dynamically important in cluster formation, and hence in modifying several key tests of cosmological theories. These researchers have been conducting simulations of cosmological evolution that for the first time include the acceleration and propagation of cosmic rays.

A third project investigates the dynamics of supernovas and the origin of cosmic rays. Supernova explosions are the primary source of the kinetic energy to the interstellar medium of the galaxy and probably the main source of galactic cosmic rays. This project has two parts. One involves a sophisticated effort to model the detailed, nonlinear physics in "collisionless" shocks thought to accelerate cosmic rays. The other involves a novel multidimensional study of the dynamics of supernova remnants in realistic environments and associated cosmic ray acceleration. The group's ultimate goal is to merge these efforts.

Victor H. Barocas, Principal Investigator

Computational Biomechanics of the Eye and of Fibrillar Tissues and Tissue Equivalents

This group's research consists of two main projects in the area of computational biomechanics. Both projects involve three-dimensional simulations that require the resources of the Supercomputing Institute.

The first project deals with coupled mechanics of the aqueous humor and the iris in the anterior portion of the eye. Pressure in the aqueous humor sets the overall interocular pressure. Elevated interocular pressure and the associated damage to the optic nerve, a condition known as glaucoma, is the leading cause of blindness in the United States. Glaucoma occurs in many different forms caused by many different underlying physiological processes.

This project is focused especially on the development of a coupled fluid-structure finite element model that describes the flow of the aqueous humor (a Newtonian fluid) and the passive deformation of the iris (an elastic solid). Initial work involving axisymmetric flow using a two-dimensional model has been able to describe some forms of glaucoma, and the group has begun to examine angle closure glaucoma, a form in which the iris is pushed forward and/or adheres to the posterior corneal surface.

Many forms of glaucoma and treatment options involve symmetry-breaking events. Specific examples include burning a hole in the iris with a laser, which is a standard treatment for certain forms of glaucoma but is not well understood, and free convection within the eye, which had been reported anecdotally but had not been documented by experiment or theory until this group's recent work. In addition, blinking is known to contribute to the contour of the iris, but the mechanism is unclear. The group is continuing to use the axisymmetric model and is also developing a three-dimensional version of the code, which will be used to solve these problems.

The second project is a novel microscopic-macroscopic finite element approach to the modeling of fibrillar tissues. The material behavior of bioartificial tissues is governed by their microstructure. However, it is unclear just how the microstructure and the properties are related, particularly in cases where the system restructures during the course of deformation. Further, although the microstructure is important, a model must be able to describe behavior on the length scale of the tissue, typically 1,000 times greater than the length scale of the microstructure; this scale imbalance presents significant challenges to the development of a useful descriptive model. This group has overcome some of these challenges and has developed a coupled microscopic-macroscopic model for tissue equivalents, which has performed well in preliminary tests. The group has improved the efficiency of the solver to the point where they can apply the two-dimensional code to real problems. They are comparing their results to the experimental data of Robert T. Tranquillo's group, which is studying the mechanics of bioartificial blood vessels and cardiovascular valve leaflets. These data, which include both mechanical and structural measurements, provide the best possible

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Victor H. Barocas, Principal Investigator

test of the model. They also, however, require the group to perform more rigorous simulations.

To this end, the group is working to add three key physical elements of the network to the model. First, physical crosslinks can occur between fibers, providing a dissipative component to matrix behavior. The exact mechanism of physical crosslinking is not well understood, so the group is developing a better understanding of the system in order to incorporate it into the model. Second, the flow of interstitial fluid, which is neglected in the current model, is known to be important in some situations and must be added. The final feature to be added, which is easier to understand but which may prove very difficult to implement, is the inability of two fibers to occupy the same space. This is a negligibly small effect in two dimensions, but may prove significant in three-dimensional systems, particularly under large compressive loads.

Mark A. Nicosia, Principal Investigator

Numerical Studies of Neurological and Cardiovascular Mechanics

This research involves two projects that are intended to enhance understanding of normal physiology, to elucidate altered mechanical behavior in pathological states, and to apply this knowledge to improve the diagnosis and treatment of disease.

The first project involves the flow mechanics of cerebrospinal fluid (CSF). The brain and spinal cord are bathed in fluid that serves as a protective barrier against trauma. During the cardiac cycle, CSF pulses as blood enters and leaves the brain. Relationships among abnormal anatomy, altered CSF flow patterns, and acquired neurological disease have been suspected, but not studied in detail. The focus of this project is to use computational fluid mechanics to help understand the etiology and improve the diagnosis of these acquired abnormalities. During this period, the researcher has developed a preliminary finite element mesh of the system that includes the spinal cord, CSF, and dura mater, and is working on simulating flow through this system.

The second project involves numerical modeling of circulatory assist devices. There are 250,000 deaths per year from heart failure. Although heart transplant is the optimal therapy for such patients, only 2,000 donor hearts are available each year. Circulatory assist devices, once seen as a bridge to transplantation, are beginning to be used as a permanent therapy. However, as these devices are implanted for longer periods, unforeseen problems have emerged, such as pathologies in the native outflow valve of the patient's heat and in the prosthetic valve of the device. This researcher is using numerical modeling to aid in understanding the cause of valvular breakdown and to optimize the design and implantation of these devices.

Robert W. Carr, Associate Fellow

Atmospheric Chemistry of the Halogen-containing Organic Compounds

This group is using Supercomputing Institute resources to complement experimental research on the atmospheric chemistry of halogenated alkoxy radicals and the chemistry of GaN chemical vapor deposition. By performing *ab initio* calculations on reactions of CF_3CClHO, CF_3CH_2O and CH_2BrO radicals, the researchers predicted optimized geometries, vibrational frequencies, and total energies of reactants, products, and transition states. The results of the *ab initio* computations are used in Rice-Ramsperger-Kassel-Marcus (RRKM) estimates of rate coefficients via molecular theories of kinetics. The researchers also used reaction path following calculations to verify that the located transition states connect with two minima in each side of the reaction coordinate (reactant and products). Comparison of the estimated and experimental rate coefficients permits development of rate coefficient models that are accurate over the entire range of atmospheric conditions, which is much wider than the range of conditions accessible by experimental methods. These calculations provide information on the effect of halogen substitution on the reactivity of these oxy radicals.

Research Group

Fuxiang Wu, Associate Researcher

In recent work, the group carried out *ab initio* molecular orbital calculations to compute geometries and vibrational frequencies of the reactant, products, and transition states of the unimolecular elimination of HCl and Cl from CH_2ClO radical at HF/6-31G(d) and MP2(full)/6-31G(d,p) levels. Total G2 and G2(MP2) energies were calculated using G2 and G2(MP2) theories. These calculations also generated the critical energies of the unimolecular dissociation reactions.

The researchers have also completed *ab initio* calculations and RRKM calculations of the unimolecular decomposition of CF_3CFHO. Optimized geometries and vibrational frequencies for reactant, products, and transition state were obtained at HF/6-31G(d) and MP2(full)/6-311G(d,p) levels. The total energies were obtained at several levels of theory up to G2(MPs).

In the study of CF_3CClHO related reactions, the *ab initio* calculations have revealed four transition states, including thermal decomposition and unimolecular eliminations of Cl, H, and HCl. In the study of CH_2BrO, *ab initio* calculations have been initiated and a transition state of Br elimination has been located. The total energies of the reactant, transition states, and products of the Br elimination are being calculated at different levels of theory, and the transition state of HBr elimination is being located.

James R. Chelikowsky, Fellow
Yousef Saad, Fellow

High-Performance Algorithms for Electronic Materials

These researchers have continued their investigations on electronic materials. These materials include dielectrics such as silica and semiconductors such as silicon, germanium gallium arsenide, and zinc telluride. A major part of this program is to develop and implement new algorithms for examining the electronic and structural properties of complex systems. Application of this research focuses on systems with numerous atoms and many degrees of freedom, e.g., surfaces, liquids, glasses, large clusters, and complex solids. This research team is also investigating dilute magnetic semiconductors, including magnetic semiconductor dots.

One project involves investigation of large clusters of semiconductors, such as silicon, which are often passivated with hydrogen atoms or similar agents. These clusters are called "quantum dots." The researchers are examining the dielectric properties of silicon in small quantum dots to construct a better description of the optical properties and electronic screening. This work entails the first realistic calculation for the full dielectric (nonlocal) response functions for localized systems. If successful, this approach will dramatically enhance the ability to examine the electronic and optical properties of confined systems. In related work, the researchers are investigating systems such as CdS and CdSe and the role of oxygen absorbed on the surface of silicon quantum dots. They have also examined small clusters of Si, Ge, GaAs, and Na, along with small molecules.

In their work on liquid semiconductors, this group has recently begun a project involving liquid silica. The goal of this research is to examine the nature of defects in silica glass.

A new area of research involves dilute magnetic semiconductors. Ferromagnetic semiconductors, especially III—IV semiconductors with a magnetic ion impurity content, have recently attracted much attention due to their potential in making use of both electron charge and spin on the same chip. In order to realize this potential, one must understand the consequences of the impurity content on the electronic structure. The researchers are investigating these systems using pseudopotentials within a spin-polarized density functional theory framework. Most of the work centers on the electronic structure of $Ga_{1-x}Mn_xAs$ and $In_{1-x}Mn_xAs$. The calculations for these systems will assume a realistic Mn content of several percent and allow for atomic relaxation results. Therefore, they allow a direct comparison to experimental data.

One of this group's long-range goals is to develop new methods for examining very large systems such as those containing hundreds or thousands of atoms. A key issue dictating the choice of algorithms is to remove any communication bottlenecks, especially when dealing with parallel architectures. The current work in this area involves exploring the use of new algorithms that do not require the computation of explicit wave functions.

Research Group and Collaborators

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Robert F. Cook, Principal Investigator

Slitting of Coating Webs

Many coated products are formed by first coating a wide (but thin) web or film and then slitting, cutting, or punching the web to yield a narrow tape or other shape much smaller than the original. Examples include such products as magnetic recording tape, which is formed of thin polymer films coated with magnetic materials, and adhesive labels, which are formed from paper multi-layer structures that are slit, cut, and punched. A general problem of the slitting process associated with these coated products is maintaining or achieving a defect-free cut edge. Such edges are crucial for yielding products that maximize the useful surface area of the slit component.

The research team's goal is to understand the slitting process so as to generate materials and process guidelines that optimize the edge quality of tapes formed by slitting. The investigation is in collaboration with Imation, which has appointed an IPrime Industrial Fellow who will implement several ABAQUS finite element models. The approach is to isolate the key elements controlling edge quality by working from the initial (web) and final (tapes) points (forwards and backwards in the process, respectively) towards the intermediate (slitting) point.

Collaborator

Raul Andruet, Imation Corporation, Oakdale, Minnesota

The plan of work includes:

- Quantifying and understanding the initial state of stress of the incoming web, as that determines the lateral curvature.
- Quantifying and understanding the force resisting film layer to fracture and delamination.
- Quantifying and understanding the driving force for film layers fracture and delamination.
- Developing an idealized "slitting" model in both two and three dimensions, including different cutting mechanisms.
- Comparing the geometry and material dependencies of the models with those observed in the slitting process.

The researchers have developed ABAQUS models of multilayer shell structures to validate their analytical expressions relating the stress field inside each layer and curvature of the composite. They have performed nanoindentation tests and developed numerical models of the nanoindentation process. They have also developed a two-dimensional finite element slitting model and are in the calibration phase, which includes the definition of the failure laws and the determination of mechanical properties in the elastic and plastic regimes. The experience gained by developing this model will be useful for the development of the three-dimensional model.

H. Ted Davis, Fellow

Simulation Studies

These researchers are involved in two simulation studies. The first is the simulation of packed-bed chromatography utilizing high-resolution flow fields. The second is simulation studies of processing and properties of surfactants in nanostructure-tailoring solvents and ions.

In the first area, these researchers have developed a computer simulation of a section of the interior region of a liquid chromatographic column that provides a detailed fluid flow profile. The fluid mechanical calculations are performed on a parallel-processor computer using the Lattice Boltzmann technique. Convection, diffusion, and retention in this flow field are calculated using a stochastic-based algorithm. This computational scheme provides the ability to reproduce the essential dynamics of the chromatographic process from the fundamental considerations of particle geometry, particle size, flow velocity, solute diffusion coefficient, and solute retention parameters when retention is utilized. The simulation data are fit to semiempirical models.

The simulations appear to capture the essential dynamics of the chromatographic flow process for nondimensional flow velocities (Peclet number) less than 500 in packed beds of monosize spheres. The best agreement is found for the "coupling" model of Giddings and the four-parameter Knox model. The researchers are interested in extending the results to polydispersed packings and to heterogeneous packed beds.

The second research project investigates salts of fatty acids, called "soaps," which comprise a class of chemicals that are of tremendous commercial importance. There is also emerging industrial interest in the crystallization behavior and nanostructure of soaps to make advanced materials of various types. Although much is known about the phase behavior of soaps in aqueous and some nonpolar solvents (e.g., propylene glycol), the kinetics of crystallization, the effects of process on the microstructure and properties of a crystallization dispersion (which is the state in which many products are used), and the origins of polymorphism (the ability of soaps to adopt different crystalline structures depending on process conditions) are not fully understood. The role of different solvents or solvent mixtures on crystal and liquid crystal formation of soaps in solution is also an important problem not yet resolved. For example, the addition of sodium salicylate to a spherical micellar solution of cetyltrimethylammonium bromide causes a transformation to a worm-like micellar solution, which can be used as an effective drag-reducing agent. Researchers do not yet have a general understanding of those transformation phenomena, however. In order to understand these issues, these researchers are performing simulation computations to augment the experimental results on the crystallization processes in various solutions subjected to various heating and cooling cycles. Combined with the theoretical techniques that have already been developed, Monte Carlo simulations are used to calculate the free energy and phase behavior of mixed amphiphiles and of amphiphile-additive mixtures, to understand the mechanism of the micellar shape transformation, and to predict the effect of the inclusion of organic additives into the micellar structures.

Research Group and Collaborators

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Jeffrey J. Derby, Fellow

Materials Processing Fundamentals

The Derby group employs large-scale numerical modeling to study several materials-processing systems. On the continuum level, these systems are characterized by nonlinear interactions between field and inter-facial phenomena. These phenomena—specifically, the transport of momentum, heat, and mass and the effects of solidification and capillarity—are analyzed via finite element computations.

On the atomistic level, the Derby group performed *ab initio* simulations (in collaboration with the research group of James R. Chelikowsky) to study phenomena that affect the microscopic properties of materials. Specific research areas included the modeling of the growth of several crystalline materials, ceramics sintering systems, the microwave heating of food, and polymer fluid mechanics.

Several topics were addressed specifically during this research period. One was the development of algorithms needed to model materials processing systems. Past work has concentrated on the development of finite element methods for solution of these problems. Work during this period focused on massively parallel implementations, the development of moving boundary techniques for three-dimensional problems, better preconditioners to be used with iterative linear solution methods, and implementation of advanced formulations for strongly nonlinear flows and transport.

In another continuing study, the team's effort has been directed at understanding several crystal growth systems. The work focuses on multi-scale models for melt and solution crystal growth systems. One such project focuses on the description of molten II–VI materials using atomistic methods to better understand their peculiar properties during crystal growth. Another project, which is being performed in collaboration with Prodromos Daoutidis, focuses on the modeling and control of the Bridgman crystal growth of cadmium zinc telluride (CZT), a chemically importation and scientifically interesting mineral. The group has finished a successful initial computation of their coupled, three-dimensional code for Bridgman crystal growth. They now plan to carry out a series of computations that will investigate the effects of ampoule tilting (a realistic imperfection caused by system misalignment) and ampoule rotation (an approach proposed to ameliorate system imperfections) during the terrestrial Bridgman growth of CZT.

Still another focus of interest for these researchers was the study of sintering phenomena. The team has successfully modeled the viscous sintering of simple configurations of particles. They are now developing a model of vacancy diffusion phenomena, which dominate the sintering behavior of crystalline materials, and extending analyses to more complicated, three-dimensional particle arrangements.

Lastly, the team studied polymer fluid dynamics in processing. The researchers developed and applied finite element methods with differential constitutive equations for viscoelastic fluids to study various flows in polymer processing. Of particular interest were polymer drop deformation and break-up in extensional and shear flows.

Research Group and Collaborators

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Modeling of Micro- and Nanoindentation of 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 values for 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.

This research project develops numerical model and viscoelastic indentation theory in support of experimental work on micro- and nanoindentation also being conducted by this group. The numerical model is expected to provide a better understanding of the mechanical properties of coating/substrate systems and the theory is to provide 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.

The researchers have previously developed two- and three-dimensional finite difference models for elasto-plastic indentation and scratch problems with large deformation. Most recently, the researchers established a two-dimensional model for viscoelastic indentation on polymers. The numerical results of this model are consistent with experimental observations. The most important characteristic from simulation of viscoelastic indentation is that the patterns of the stress field during the period of stress relaxation are the same, although the amount of stress level is reduced. In comparison, the elasto-plastic indentations have different patterns of stress field at loading and unloading steps. Another feature of the simulation is that the load-drop reaches 30% of total load after the material experiences a complete stress relaxation. This feature is in good agreement with the experiments. This has helped the researchers understand the viscous material mechanism as well as probe properties of polymers. Therefore, the researchers believe that the model will assist them to apply indentation techniques more efficiently for the merging polymers. The next step is to thoroughly test the model and validate it with experimental data.

Research Group

Liangsheng Cheng, Research Associate

Wei-Shou Hu, Associate Fellow

Mechanistic Study of Hepatocyte Spheroid Formation

Researchers use confocal microscopy to observe the self-assembly of hepatocytes into spheroids. The out-of-focus information and noise caused by optics and electronics results in artifacts and impedes further data analysis and volume reconstruction. These researchers have implemented parallel iterative deconvolution to process confocal micrographs of hepatocyte spheroids and use this to visualize the cells during the spheroid formation process.

Different states during the course of spheroid formation are characterized by differing patterns of gene expression. One promising analysis method is carrier deoxyribonucleic acid (cDNA) microarray analysis of gene expression profiles, in which labeled cDNA is incubated on a DNA microrray containing thousands of spots, each corresponding to a unique DNA sequence. The fluorescence intensity of a spot is assumed to be proportional to the initial concentration of the corresponding DNA in solution. Labeled DNA species have to diffuse in solution to the corresponding spot and undergo a second-order hybridization reaction with the immobilized DNA.

This group has developed a kinetic model for the hybridization process that considers the dynamics of diffusion of labeled cDNA strands and duplex-formation reactions. They use finite element analysis to numerically solve the partial differential equations that arise from the modeling. The aim of the modeling study is to formulate strategies for maximizing the ratio of true to false positive fluorescence intensity for species with varying abundance levels and varying degrees of regulation. The model predictions will be compared with results of hybridization experiments using the defined concentration and identity of labeled cDNA species.

These researchers have also begun a new line of investigation, modeling regulatory networks and cell metabolism from a global perspective. Cell metabolism is essentially a complex network of reactions with many enzymes and reactants as well as regulatory networks controlling the expression of both regulatory elements and the biochemical network. The regulatory network consists of a large number of regulatory elements of interacting genes and proteins organized in hierarchical trees. Cellular events involve the interplay of these elements of the regulatory network.

The Hu group has developed an algorithm based on a Boolean framework to reverse engineer the network. The algorithm's performance was evaluated using a set of synthetically generated networks as well as an actual network derived from the yeast cell-mating pathway. They have generated a number of different networks with genes varying from 10 to 100 and with varying in-degree. Exploring the entire possible network space demands a great deal of computing power and the problem quickly scales up with the number of nodes, so the resources of the Supercomputing Institute are necessary for this research.

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Computer Simulations of Model Lung Surfactants

Pulmonary surfactant (PS) is a surface-active phospholipid-protein material that lines the alveolar epithelium. It reduces the surface tension at the air/water interface, stabilizing the alveoli during expiration. Deficiency of pulmonary surfactant results in respiratory distress syndrome (RDS) in premature infants. Since supplies of human lung surfactant are extremely limited, a typical treatment of RDS involves the use of animal surfactants as a replacement for human PS. However, animal sources carry the danger of viral infection or immunological response. Thus, developing a synthetic lung surfactant is an important research goal.

The main phospholipids and principal tensoactive components of PS are phosphatidylcholine (PC) and phosphatidylglycerol (PG). PC and PG reduce the surface tension throughout the lung and contribute significantly to the lung's compliance. The surfactant proteins SP-B and SP-C also enhance the surface properties of the surfactant. As a first step toward understanding how surfactant function is affected by the component interactions, these researchers are investigating the morphology of monolayer films of dipalmitoylphosphatidycholine (DPPC), dipalmitoylphosphatidylglycerol (DPPG) and SP-B(1-25) at the air/water interface. These model systems have been extensively investigated with experimental techniques and are thought to adequately describe *in vivo* surfactant function phenomena. This research uses CHARMM (Chemistry at Harvard Macromolecular Mechanics) on the SGI Origin 3800.

During this period, the researchers have run a number of simulations with the lipid monolayer in the absence of the peptide. Specifically, they conducted atomistic molecular dynamics simulations of DPPC and DPPG monolayers at the air/water interface. The simulations are carried out at different surface densities and a simulation cell geometry is chosen that greatly facilitates the investigation of phospholipids monolayer properties.

A new project for this group involves the *in silico* prediction of protein structures. The determination of protein structures is a key step toward understanding the behavior of biomacromolecules and initiating knowledge-based, rational approaches for engineering molecular solutions. Experimental efforts such as x-ray crystallography and nuclear magnetic resonance techniques are not efficient enough to allow for rapid structural determination of the ever-increasing number of newly discovered sequences. Hence, computational, theoretical methodologies are becoming essential to protein sequence/structure/function relationship research. In this project, the Kaznessis group plans to develop and implement novel, integrated information technology methodologies for recognizing the fold of proteins, based largely on the discovery of non-local interactions. Many algorithmic procedures in the areas of computational biology, machine learning, computational geometry, data mining, and graph theory are being developed that create an integrated information technology approach, which will enable researchers to accurately and efficiently assign folds and functionalities to novel protein sequences.

Research Group

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Satish Kumar, Principal Investigator

Three-dimensional Simulations of Viscoelastic Fluid Flow in a 4:1 Concentration

The goal of this research project is to solve the equations governing the flow of a viscoelastic fluid in a 4:1 planar contraction. Simulation of viscoelastic fluid flows is of considerable practical importance because many polymeric and composite materials exhibit viscoelastic rheological behavior. These problems are notoriously difficult due to the highly nonlinear relationship between stress and strain. The 4:1 planar contraction is a model problem that these researchers are examining in order to validate a code they have recently developed. Using stabilization techniques such as fractional step method (FSM) and discrete elasto-viscous split-stress gradient/streamline upwinding Petrov Galerkin (DVSS-G/SUPG), the researchers obtained stable numerical solutions up to high Weissenberg number (*We*—the ratio of the fluid relaxation time to a characteristic deformation rate), and were able to observe a vortex enhancement process. This process was the merging of the corner and lip vortices. The constitutive model used was the Oldroyd-B equation.

The simulations also showed that the evolution of the vortex cores of the transient solution follows that of the steady-state solutions at different *We*, which means that there may exist a strong relationship between time in the transient state and the Weissenberg number in the steady states. If such a relationship holds, it may well be applicable to more complex viscoelastic flows and could help in understanding their behavior. Because this result may be a numerical artifact of the two-dimensional simulation, the researchers are developing a three-dimensional model. This work will establish a benchmark for three-dimensional simulations of viscoelastic fluids, and, more generally, will yield deeper insight into their fascinating flow behavior.

Collaborators

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Intermolecular Potentials Inferred From Crystallographic Data

Molecular crystals are of interest for a wide range of applications. Crystallization is a highly selective separation method used to purify pharmaceuticals. Molecular crystals are also being investigated for use as optical and electronic materials. In each of these applications, the molecular arrangement within the crystal structure determines its properties. Often there are multiple structures, called polymorphs, with differing properties. Methods to identify and to select desirable polymorphs are needed to replace current trial-and-error methods.

Crystal structure prediction is notoriously difficult because multiple polymorphs may have similar free energies and identifying the most stable crystal is very sensitive to the intermolecular potential parameters. This group is putting this extreme parameter sensitivity to their advantage. Since small perturbations of the intermolecular potential change the most stable crystal structure, the existence of a particular structure implies stringent constraints on the intermolecular potential. Delineation of the family of intermolecular potentials consistent with an observed crystal structure is what this group calls reverse engineering of the crystal. They are using the Cambridge Structural Database to identify structures and phase transitions for a group of tetrahedral molecules as a test of their methods.

Research Group

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Alon V. McCormick, Fellow

Molecular-Scale Chemical Reaction Engineering of Materials Synthesis

Molecular-scale models are used to characterize chemical engineering systems that pose special process modeling difficulties because they are governed by poorly understood molecular-scale interaction. During this research period, the McCormick group was involved with three major project areas using molecular-scale models:

- Percolation simulation of crosslinking polymerization.
- Computer simulation of viscoelasticity and solidification of curing coatings.
- Simulation studies of processing and properties of surfactants in nanostructure-tailoring solvents and salts.

Free-radical polymerization of multifunctional monomers such as (meth)acrylates leads to the formation of highly crosslinked polymer networks. These networks have found applications in coatings, films, information technology, and other areas. Such crosslinking polymerization exhibits special features, however, which are not observed in linear polymerization. These features include unequal reactivity of pendant and monomeric functional groups, microgel formation, and structural heterogeneity. To characterize these features, this group is developing a lattice percolation model.

The microscopic structure of a linear viscoelastic material is mechanically equivalent to a network of linear viscous and elastic elements. The elements considered in this analysis are "springs" that represent elastic deformation, and "dashpots" that represent viscous-like changes in the stress-free state. Each element is joined at each of its two

Continued on next page

Alon V. McCormick, Fellow

ends to one or more other elements. The node-element incidence matrix method is used to model the force balance in the network. An incidence matrix is defined that incorporates the connectivity of the entire network. The equation governing the stress development is then given by a differential algebraic equation that can then be solved for time to obtain the changing stress state in the system. The researchers have modeled this equation and have gained insight into understanding viscoelasticity in a network.

A network of springs and dashpots can also be used for modeling curing coatings. The monomer is represented mechanically by a network of dashpots. A dashpot is replaced with a spring every time a bond forms. Thus, elasticity in the network builds as the network cures. The goal is to study the evolving viscoelasticity in the curing coating and to track the stress development. This model will be combined with the kinetic gelation modeling described above. This will allow the researchers to optimize the curing process in order to maximize conversion and minimize stress.

The researchers have also begun studies to understand wrinkling of coating surfaces. This will involve modeling of the stress in the coating and some instability studies of the coating surface.

The McCormick group is also studying salts of fatty acids ("soaps"), which comprise a class of chemicals that are of tremendous commercial importance. There is also emerging industrial interest in the crystallization behavior and nanostructure of soaps to make advanced materials of various types. Although much is known about the phase behavior of soaps in aqueous and some nonpolar solvents (e.g., propylene glycol), the kinetics of crystallization, the effects of process on the microstructure and properties of a crystallization dispersion (which is the state in which many products are used), and the origins of polymorphism (the ability of soaps to adopt different crystalline structures depending of process conditions) are not fully understood. The role of different solvents or solvent mixtures on crystal and liquid crystal formation of soaps in solution is also an important problem not yet resolved. For example, the addition of sodium salicylate to a spherical micellar solution of cetyltrimethylammonium bromide causes a transformation to a worm-like micellar solution, which is an effective drag-reducing agent. However, there is no general understanding of these transformation phenomena.

In order to understand these issues, the McCormick group has performed simulation computations to augment experimental results on the crystallization processes in various solutions subjected to different heating and cooling cycles. Combined with the theoretical techniques already developed (free energy models), they used Monte Carlo simulations to calculate the free energy and phase behavior of mixed amphiphiles and of amphiphile-additive mixtures, to understand the mechanism of the micellar shape transformation, to provide molecular detail of the micelles (such as the intra-micellar order), and to predict the effect of the inclusion of organic additives into the micellar structures.

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Computational Polymer Physics

These researchers are interested in computational polymer physics, which focuses on elucidating molecular origins of both equilibrium and dynamics behavior of polymer fluids. The group investigated two areas:

- Statistical dynamics and viscoelastic behavior of solutions of semi-flexible polymers, studied by Brownian dynamics simulation.
- Statistical thermodynamics of self-assembling structures of block copolymers, studied by a self-consistent field theory.

In the first area, the researchers are carrying out a program of Brownian dynamics (BD) simulations of Brownian motion and viscoelasticity of solutions of semi-flexible polymers. The simulations are tightly integrated with theoretical investigations of such solutions. The simulations use a worm-like chain model that describes a polymer as a continuous contour with an elastic resistance to bending and a constraint prohibiting longitudinal compression or extension. Among the molecules that are well described by this model are many biopolymers, including deoxyribonucleic acid, collagen, and cytoskeletal filaments such as actin, as well as many synthetic polymers that exhibit a nematic liquid-crystalline phase in solution, such as Kevlar. Recent work has focused on developing a code for interacting polymers. These simulations use a model of semiflexible bead-rod chains with constrained rod lengths (like the single chain simulations), which interact with rod-rod (rather than two-body bead-bead) repulsive interactions in a period unit cell. The initial version uses a linked-cell list to identify near neighbors. The first version of the code simulates a solution of uncrossable but infinitely thin line-like polymers, using an algorithm based on a geometrical criterion that prevents chains from crossing. The algorithm is being refined and used for simulations of equilibrium dynamics in entangled solutions.

The second research area centers on the use of self-consistent field theory to calculate the structures, free energies, scattering profiles, and elastic moduli for periodically ordered phases of block copolymers. The researchers are working on the calculation of structure and phase diagrams for triblock copolymer melts, especially concentrating on calculating the structure and free energy of a new non-cubic multicontinuous morphology. They have recently finished work on the calculation of elastic moduli of three dimensionally periodic body-centered-cubic and gyroid ordered phases of di-block copolymers, as functions of relative volume fractions of the two phases and temperature. In the process of solving this problem, the researchers have solved a series of algorithmic challenges, including the development of a much more efficient iteration algorithm and, recently, the development of a FORTRAN 90 crystallography module that allows them to generate basis functions appropriate to the simulation of structures with any of the 230 possible crystallographic space groups.

Research Group and Collaborator

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Two-dimensional Millisecond Reactor and Catalytic Radiant Burner Modeling Using Detailed Chemistry

Millisecond, adiabatic reactors used for the partial oxidation of alkanes to synthesis gas (syngas), olefins, and oxygenates have been extensively studied for chemical manufacture for CO-free hydrogen streams for fuel cells. This research group is studying the partial oxidation of alkanes to syngas and subsequent shift of CO to CO_2 to obtain low CO hydrogen streams on noble metal catalysts in millisecond tubular reactors. A major focus has been the partial oxidation of ethane to ethylene, as well as catalytic wall reactors that couple exothermic reactions with endothermic reactions in order to eliminate thermal boundary layers. All of these projects involve coupling reaction kinetics with complex fluid dynamics to obtain models to describe these processes.

Surface mechanisms for partial oxidation are constantly being updated. To accurately describe this system, water-gas shift and methantion kinetics are being added into the mechanism in order to describe the addition of steam into the system. FLUENT is used to couple catalytic surface reactions, heat transfer, and fluid dynamics in order to describe the millisecond reaction in two dimensions. Further work is being carried out to describe the light-off of the rhodium catalyst. This is a first step in describing the transient temperature and product profiles for the fast start-up of millisecond reactors.

Surface mechanisms are also being updated for the oxidative dehydrogenation of ethane to ethylene. The CHEMKIN model, which contains 40–100 heterogeneous reactions along with 450 gas phase reactions, describes product profiles in the millisecond reactor. Further work involves incorporating the mechanisms from CHEMKIN into FLUENT to capture the fluid dynamic behavior as well as the reaction and heat transfer behavior.

The researchers have started simulations in CFD-ACE along with on-going FLUENT simulations in order to model the catalytic wall reactor. In this reactor, platinum is coated on one side of a wall to combust methane and create large amounts of heat. The other side of the wall is coated with rhodium to catalyze the steam reforming of methane in order to produce hydrogen. This reaction is highly endothermic and uses the heat generated on the other side of the wall to sustain itself. The presence of the reactions on the walls leads to the absence of thermal boundary layers at the walls, which would be present if these reactions were to take place in the gas phase. CFD-ACE and FLUENT are used to couple the fluid dynamics, heat transfer, and heterogeneous chemistry to better characterize this system.

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Physics of Fluids in Processing Technologies

This group performed pioneering research into computational aspects of continuum and network theories of fluid physics and transport in film and in porous media structures.

This work was a part of coordinated research programs on the fundamentals of liquid structure, flow, and transport in commercially important process technologies, such as precision coating, drying and curing of liquid films, injection molding, and multiphase contacting in packed beds. The problems are typically multidimensional and frequently time-dependent, resulting in systems of coupled partial differential equations that are solved using finite element techniques with Newton iteration and parametric continuation for mapping of the solution space. The stability of these solutions—which leads to eigenanalysis—as well as their response to small sinusoidally forced disturbances is also important. To obtain comprehensive results, the basic problem must be solved many times; this demands the speeds offered by high-end workstations or massive parallelization capabilities of the same. For the majority of the problems solved, the size is 5,000–15,000 unknowns per single steady state solution, though very large two-dimensional and three-dimensional problems are occasionally needed.

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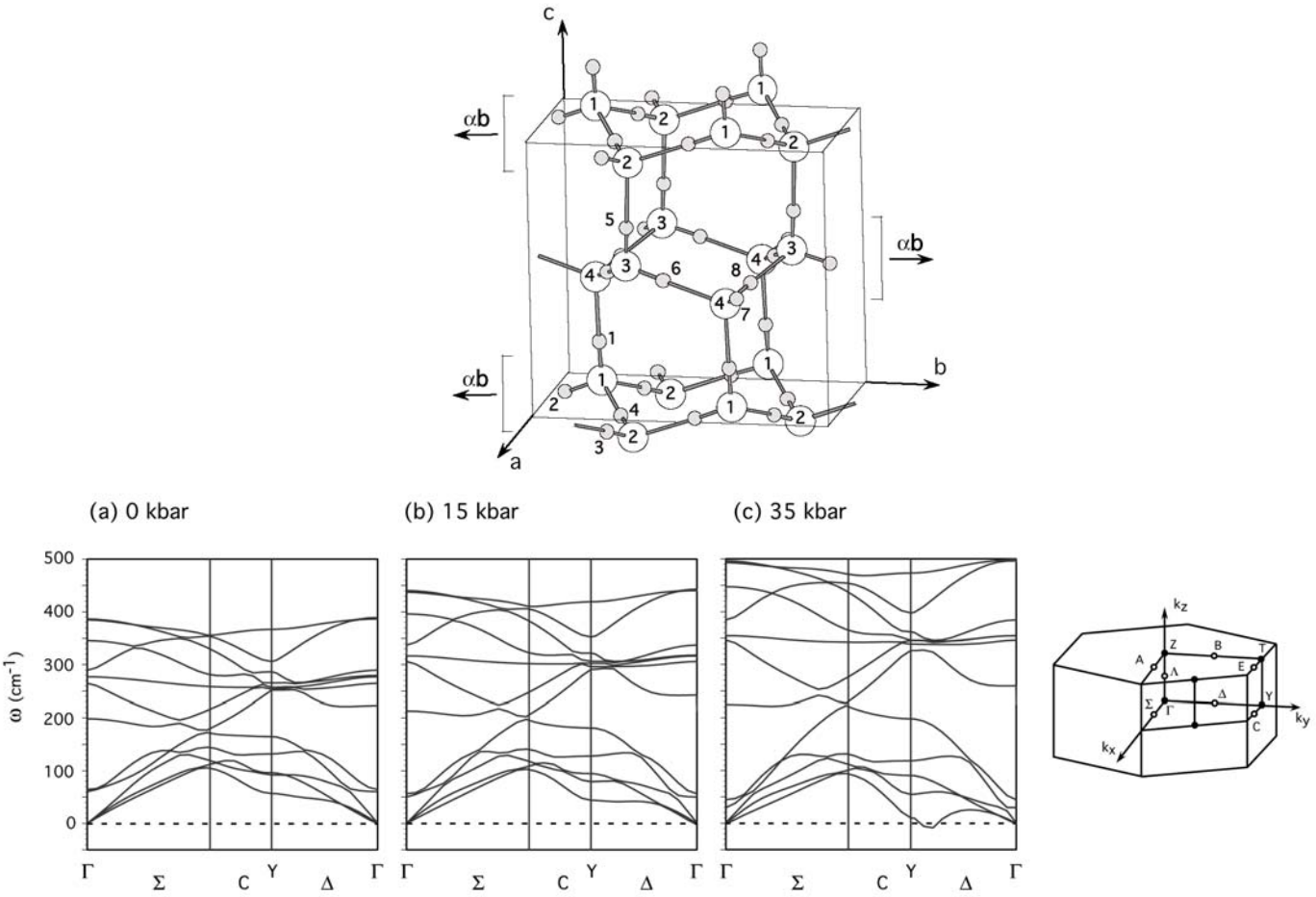
Renata M. Wentzcovitch, Fellow

Elastic and Structural Properties of Minerals at Planetary Interior Conditions



Prediction of an incommensurate phase transition in ice XI. *(Top)* Structure of ice XI. *(Bottom)* Phonon dispersions at 0, 15 and 35 GPa. The negative values correspond to imaginary frequencies. This transformation should be the precursor of another phenomenon: complete amorphization of the ice XI structure (by Dr. Koichiro Umemoto, submitted to *Physical Review Letters*).

Research in the Wentzcovitch group is devoted to quantum mechanical studies of materials. The first principles methodology used is based on Density Functional Theory (DFT) and Pseudopotentials (PP). DFT-PP-based methods do not rely on any *a priori* information about the material, except the fundamental constants of nature and the atomic numbers of the elements. Yet they are predictive beyond the current limits of many kinds of experiments. This is particularly true of matter subjected to extremely high pressures and/or high temperatures (P,T). First principles molecular dynamics (MD) and lattice dynamics (LD) are powerful complementary methods used to address thermodynamic properties of matter at the extreme conditions encountered throughout the solar system, such as those in planetary interiors and surfaces.

One major effort is dedicated to the understanding of the thermo-chemical state of the

Renata M. Wentzcovitch, Fellow

Earth's mantle, traditionally divided into upper mantle (UM) (down to 410 km depth), transition zone (TZ) (from 410 to 670 km depth), and lower mantle (LM) (from 670 to 2,898 km depth). Although there is a consensus today regarding the mineralogy of the UM and, to a lesser extent, the TZ, no samples are available from the LM. This region is remotely probed by seismic tomography, which offers three-dimensional maps of seismic velocities and density. From these, the elastic properties of the mantle can be extracted. Interpretation of this information in terms of temperature field and mineralogy depends entirely on the comparison of this information with the independently determined elasticity of candidate mineral phases and their aggregates (rocks). The Wentzcovitch group is pursuing high P,T elasticity calculations of possible LM aggregates to help unravel the thermo-chemical state of this region.

Hydrogen is the most abundant element in the universe and oxygen the most abundant element in the terrestrial plants. Not surprisingly, solid water is one of the most abundant solids in the solar system. The P,T regime throughout the solar system invites a wealth of solid structures, some ordered, some only partially ordered, others fully disordered. To date, more than twelve crystalline phases have been identified to the Mbar pressure regime, not all being fully ordered or stable. The stability field of these phases is not well characterized, the reason being the large amplitude of the hysteresis loops. Two other related phenomena are the negative Clapeyron slope for the melting transition of ice Ih, and the low P form of ice and its pressure-induced amorphization. This rich phenomenology is apparently unmatched by other solids. These researchers are currently investigating pressure-induced amorphization in ice and some structural systematics in P,T space. Pressure-induced amorphization was discovered in ice Ih under pressure, but it has been observed in several materials, some of which the group has investigated in the past (silica and BAs).

Finally, the group is interested in investigating the magnetic state of materials at low temperatures. Magnetism, to a great extent, is a phenomenon still better investigated experimentally. It is a low-energy phenomenon that demands high accuracy from first principles methods. Nevertheless, experiments can derive many insights and guidance from first principles theory in search of new effects. For instance, there are intriguing magneto-structural effects, and the researchers are interested in their exploration by using pressure. However, the group's main interest is the investigation of conductive materials where there exists a strong relationship between magnetism and transport. They are particularly interested in potentially novel half-metal systems, such as CoS_2. This research is inspired by and assists the experimental effort on magnetic heterostructures at the University of Minnesota.

Research Group and Collaborators

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Koichiro Umemoto, Research Associate

George Barany, Principal Investigator

Design and Characterization of Biomolecules

The engineering of stable folded and functional biomolecules has recently attracted much research attention. Within this field, the Barany group is particularly interested in the design, synthesis, and characterization of protein core modules and cyclic peptic 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 and/or B1 immuno-globulin binding domain linked by natural or designed sequences, and they contain a strategically placed cross-link to limit conformational space to more collapsed conformations. The studies carried out by these researchers exemplified new approaches 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. The Barany group is designing cyclic PNAs 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, requiring the resources of the Basic Sciences Computing Laboratory. Once the designed molecules are synthesized, they will be studied with nuclear magnetic resonance spectroscopy, from which structural features can be calculated.

Research Group

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Judit Tulla Puche, Graduate Student Researcher
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David A. Blank, Principal Investigator

Studies of Excited State Proton Transfer

These researchers continued their investigations of the excited state intra- and intermolecular proton transfer, in 2-(2-pyridyl)pyrrole (PP) in solution. This system serves as a model for intra- and intermolecular proton transfer with nitrogen atoms as both the proton donors and acceptors. This project included four aspects:

- Study the effects on both the proton transfer energetics and the spectroscopic properties of adding a variety of different substituents to both the pyrrole and pyridine rings. These studies include the effects of solvation using the CM2 charge model and SM5.42 solvation model.
- Address the equilibrated excited state at a higher level of theory than previously used.
- Consider the addition of a hydrogen-bonded cyclic bridge that can mediate a concerted proton transfer with the inclusion of a water or alcohol molecule as the bridge.
- Investigate the energetics of forming a dimer, and calculate the energetics of a double intermolecular proton transfer within a hydrogen-bonded dimer.

The calculations have supported the group's experimental, nuclear magnetic resonance, and fluorescence spectroscopy investigations of the PP system. They have examined the structure and energics of the system in both the gas and condensed phases. Based upon those results and those of related systems, the researchers have construed that the observed spectroscopic behavior of the pyridyl pyrrole system is due to complexation of the molecule with alcohol. The cyclic bridged pyridyl pyrrole alcohol complex facilitates an excited state double intermolecular proton transfer.

These researchers are now continuing their investigations of excited state proton transfer with a study of the intramolecular proton transfer in 1-(acylamino)anthraquinones. Proton transfer has been experimentally observed in this system on a femtosecond time scale, and based upon the acyl group the rate of the proton transfer may be varied. In conjunction with their ultrafast spectroscopic experiments, these researchers are beginning to investigate the energetic and structural aspects of this event with respect to the acyl group as well as evaluating the role of the solvent in the proton transfer. The researchers will model their system using a variety of semiempirical and *ab initio* methods. Vertical excitation energies and solvation effects are also being examined.

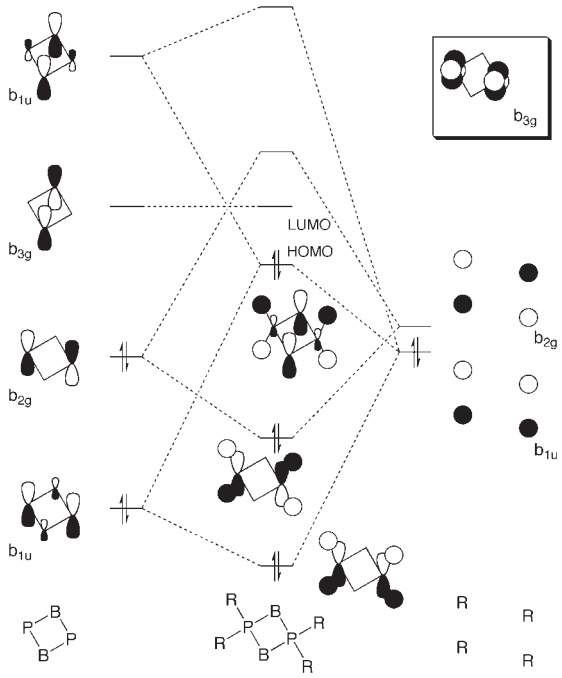
In addition to the continued energetic and structural evaluations, the researchers are beginning molecular dynamic simulations of their model systems with the goal of comparing these simulations directly with their ultrafast experiments. Based upon pre-established methods, they are modifying a molecular dynamics code to model their experimental measurement. The eventual aim of this project is to provide a theoretical comparison for experimental analysis of not only proton transfer model systems, but of all the condensed phase systems under investigation in the Blank laboratory.

Research Group

Sarah Schmidtke, Graduate Student Researcher

Christopher J. Cramer, Fellow

Computational Chemistry



LUMO: Lowest unoccupied molecular orbital
HOMO: Highest occupied molecular orbital

Molecular orbital diagram of the mixing of diphosphadiborete p orbitals with symmetry-adapted substituent orbitals on P (e.g., 1s orbitals for R = H or sp3 orbitals for R = alkyl or silyl). Inset at upper right is a b3g combination of *d* orbitals that could hybridize with and lower the energy of the LUMO if P were to be replaced by an early transition metal.

These researchers are involved in a wide variety of modeling studies. Focus areas include:

- Predicting the dynamical properties of ribonucleic acid (RNA) and deoxyribonucleic acid (DNA) tetraloops.
- Including solvation effects in quantum chemical calculations.
- Calculation of accurate multiple splittings in open-shell systems.
- Understanding the structure and reactivity of phosphorus-containing molecules.
- Characterization of organometallic systems with respect to structure and reactivity.

One area of study for the Cramer group is the enzyme tyrosinase. This enzyme is responsible for hair color and fruit discoloration. Tyrosinase has an active site with two copper atoms and is noteworthy for its use of molecular oxygen as a source of oxidizing power. The reaction catalyzed by tyrosinase is the oxidation of phenols (in the biological form of tyrosine) to catechols, which polymerize to colored materials. Besides the economic interest in the actual reactions of tyrosinase, the enzyme is of fundamental interest because it sheds light on related systems, including the photosynthetic active site (which activates molecular oxygen in a similar way, albeit with manganese metal atoms) and organometallic catalysts for C–H bond activation. The mechanism of tyrosinase itself is rather poorly understood, and there is debate in the literature about the nature of the reaction path and the rate-determining step along that path. As the active site has six histidine residues in the vicinity of the copper atoms, there is also some controversy about the ligation (six vs. four vs. other numbers of histidine ligands). The Cramer group has begun a careful study of the complicated reaction path with the goal of surveying ligands of varying numbers and donicities to better understand their influence on the reaction path. Thus, they are examining no ligands at all, and combina-

Christopher J. Cramer, Fellow

tions of from one to six ammonia, imidazole, and hydrogen cyanide ligands. Initial studies indicate that the ligands play an important role in lowering the reaction barriers and affecting the preferred pathway. These calculations are extraordinarily demanding because the electronic states of the dinuclear systems are best described as weakly antiferromagnetically coupled singlets. These require that quadratically convergent self-consistent-field schemes be used to converge the wave functions in a stable fashion. This requirement, together with large one-electron-basis set requirements, creates a demand for Supercomputing Institute resources.

In another project, the Cramer group is using principle components analysis of DNA motion (sometimes called "essential dynamics") to attempt to analyze the relative utility of positional autocorrelation functions, root-mean-square deviation analysis, and conformational entropy as measures of molecular relaxation times and convergedness. At present, they are working with a 20 ns simulation of a DNA dodecamer, which implies a data file of roughly 20 million snapshots of a system containing several thousand atoms. Data analysis is proceeding. The researchers have also carried out a less time-consuming analysis on a double-helical RNA oligomer to evaluate how base-pair mismatches affect its essential dynamics. The group is also studying variants of a structurally characterized (by nuclear magnetic resonance) alanine transfer RNA (tRNA) using a tetraloop analog. The simulation includes the full environment (water, counterions, etc.) and takes advantage of recent advantages in simulation technology (for example, parallel simulation code and particle Mesh Ewald accounting for long-range electrostatics). Moreover, they are using experimental data for a mutant version of the tetraloop known to have different properties with respect to charging the RNA with alanine and are comparing the dynamic behavior of the two in simulations in order to understand their different biological activity. A new effort in this area is aimed at modeling the recognition and editing activity of an aminoacyltransferase when its cognate tRNA is mischarged. This modeling of a protein/RNA hybrid stresses the limits of current computational methods and technology because of its size and complexity. The researchers are also modeling the effect of C:U mismatches on simulations of DNA dodecamers to better understand the dynamic timescales associated with polyelectrolytes and their fundamental motions as analyzed by principal components analysis.

Research Group and Collaborators

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Design of Semisynthetic Enzymes Based on Fatty Acid Binding Proteins

The objective of this research project is to develop 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 deoxyribonucleic acid (DNA) methods. The ability to prepare such catalysts could have a significant impact on the manufacture of a wide variety of specialty chemicals.

The specific aims of this project are to:

- Improve the efficiency and control the specificity of transaminating catalysts based on protein cavities using site-directed mutagenesis.
- Assess whether changes in cofactor structure can be used to modulate the properties of transaminating catalyst based on protein cavities.
- Expand the chemistry that can be performed using protein cavity based catalyst to include C–C bond formation.

Research Group

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Computer Simulation of Chemical and Biochemical Systems

This research group is performing investigations in several areas of chemical and biological interest. The goal of these projects is to develop computational methods and to then apply these computational techniques. The researchers use combined quantum mechanical and molecular mechanical (QM/MM) approaches in molecular dynamics and Monte Carlo simulations to model these systems.

The researchers are addressing four areas:

- The dynamics and mechanism of enzymatic reactions.
- The structure and interactions of membrane proteins.
- Modeling protein-protein interactions.
- Solvent effects on chemical reactions and interactions in condensed phases.

The first project involves molecular dynamics simulations of enzymatic reactions including the dephosphorylation reaction of human protein tyrosin phosphatase 1B (PTP1B), hydrogen transfer reactions catalyzed by the enzymes of dihydrogolate reductase, acyl-coA dehydrogenase and transketolase, cathepsin K, and the squalene to hopene conversion by squalene cyclase. In addition, the researchers are investigating the vibrational population relaxation of an azide ion in the active site of carbonic anhydrase II. These studies will provide a deeper understanding of enzyme-substrate interactions and can help to better design cholesterol-lowering drugs and therapeutic agents for treatment of cancer, diabetes, and obesity.

The second project is aimed at the prediction of three-dimensional structures of membrane proteins by making use of nuclear magnetic resonance results, and at the understanding of protein-lipid membrane interactions. This is a new project area for this group, but the computational details are similar to a prior study of the protein Bacteriorhodopsin. The researchers are also interested in the theoretical study of processes involving electronically excited states in proteins. These include the effects of mutation on spectral tuning of rhodopsin and photoactive yellow protein, a sensory protein.

The third research area is an exploratory study to model protein-protein interactions and protein diffusion in a cellular environment. It is a collaboration with George Karypis, Computer Science and Engineering Department.

The final project focuses on novel computational techniques in combined QM/MM calculations and applications to modeling solvent effects on SN2 reactions and the choice of geometrical and energy-gap solvent reaction coordinates in potential of mean force calculations. This project also aims at developing novel potential energy functions for biomolecular simulations.

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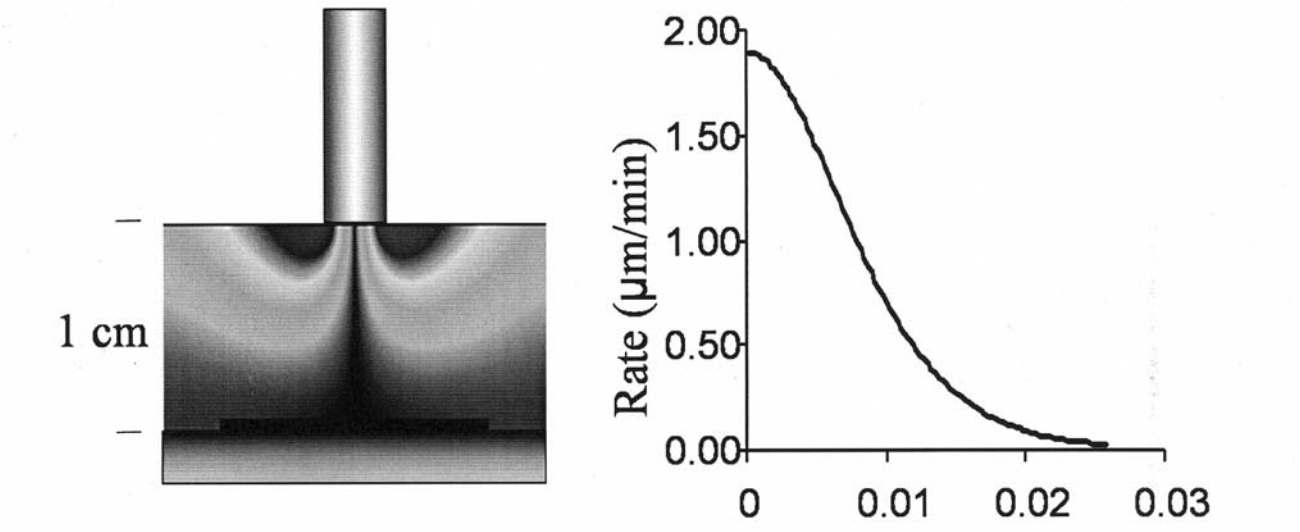
Finite Difference Modeling of Reduced Pressure-Chemical Vapor Deposition Processes



Flow streamlines in an exisymmetric reactor using $Ze(O^tBu)_4$ in N_2 impinging on a substrate having T = 400°C (left). Predicted growth rate as a function of position (right).

These researchers are using the CFD-ACE software package to create finite difference models of chemical vapor deposition processes at reduced pressures. The product of these simulations will contain information about deposition rates at various points in an axially symmetric reactor. Different precursor gas flow rates and reactor background pressures are being investigated to give information about the spread of the molecular precursor on the substrate surface and the profile of film deposition for each set of conditions.

The Gladfelter laboratory is using a novel chemical vapor deposition molecular precursor gas jet configuration to create metal oxide films with locally variable compositions for rapid screening of new high *k* dielectric materials for semiconductor applications. Precursor gases are introduced to the substrate by the use of metal dosing tubes that each deliver a dose of molecular precursor in close physical proximity to the substrate. This close proximity creates a non-uniform material composition across the substrate sample that allows rapid analytical investigation of many material combinations on a single substrate sample. This combinatorial approach to new materials development is aided by computer simulations of deposition profiles at various precursor flow rates and reactor background pressures. The simulation results will be used to assist in choosing appropriate reaction conditions to maximize the compositional variability in the combinatorial thin film samples. This will create the most effective screening process for the investigation of large stoichiometric spreads of combinations of various metal oxides.

Research Group

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Thomas R. Hoye, Principal Investigator

Computation of Proton and Carbon NMR Chemical Shifts

Nuclear magnetic resonance (NMR) spectroscopy is the single most powerful spectroscopic tool for determining the three-dimensional structure (i.e., stereostructure consisting of the relative and absolute configurations of the molecule) of organic compounds, including the important subset of natural (and unnatural) products having useful biological activities. The precise stereostructure imparts the biological function to such compounds. Thus methods for determining their unambiguous stereostructure are of considerable value. The Hoye group has begun to develop new methodologies that involve the comparison of computed with experimental spectroscopic parameters. The two principal features at the very core of nearly all NMR spectroscopic analyses are chemical shifts (∂) and coupling constants (J). These researchers have experience and success applying the Js to interesting structural problems.

In the Hoye laboratory, NMR spectroscopic techniques, in conjunction with molecular studies, have been used to assign relative stereochemistry in the case of the ottelione class of compounds. In this approach, empirically determined coupling constants are compared with computationally determined coupling constants derived from the subset of lowest-energy conformers for each possible diastereomer. While this method is both powerful and reliable, there are limitations: spectroscopic correlation can only be made between diastereomerically discernable atoms; complex and higher order coupling can convolute spectroscopic interpretation; and, since the number of diastereomers increases exponentially with the number of chiral centers (i.e., 2^n), additional stereocenters greatly increase computational costs and decrease computational feasibility. Popular commercially available software has achieved some success in predicting NMR chemical shift and coupling constant data. However, the algorithms employed do not effectively address the effects of altering the relative stereochemistry. Large differences in proton and carbon chemical shifts, ∂, often occur as a function of the local stereochemical environment.

The Hoye laboratory is now exploiting the ∂s. The new hypothesis is: comparison of computed chemical shifts for each member of a family of possible stereoisomers with the experimental chemical shifts for a single stereoisomer for which the relative configuration is not yet known, will allow the configuration of that compound to be deduced with confidence.

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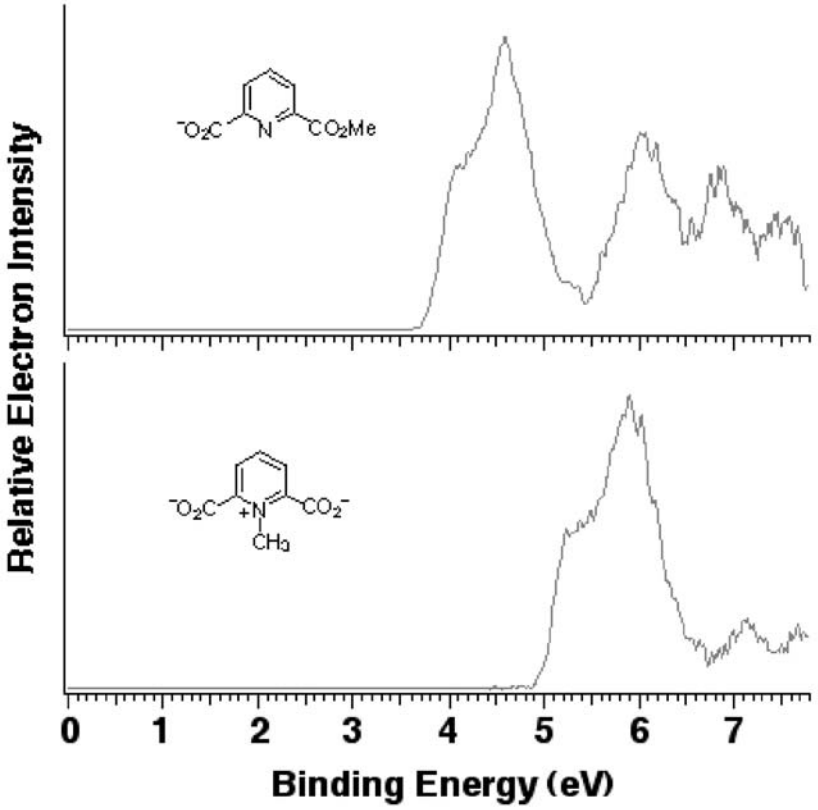
Understanding Organic Systems via Molecular Orbital Calculations



Photoelectron spectra of a zwitterion (bottom) and its "neutral" analog (top).

The Kass research group used supercomputing resources to carry out *ab initio* molecular orbital and density functional calculations on a variety of organic systems. The group is especially interested in reactive intermediates (key intermediates in numerous chemical and industrial processes), antiaromatic compounds (potential substrates for the design of novel materials), and zwitterions (important species in biological processes). These results aided in the design and interpretation of experimental data.

In their research on reactive intermediates, these researchers have 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 causes different radical anions to form. As anions and radical anions can be used to obtain quantitative thermodynamic information on the corresponding species with one fewer electron, the researchers are then in a position to interrogate a

Research Group and Collaborator

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Steven R. Kass, Associate Fellow

whole "treasure trove" of transient, but highly important, molecules.

The Kass group is also studying antiaromaticity. Aromaticity and antiaromaticity are familiar and important concepts known to all chemists. Numerous examples of compounds with the former quality have been reported, while antiaromatic species have proven to be elusive and difficult to generate. This group has previously synthesized a substituted cyclopropenyl anion, the prototypical antiaromatic species. 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.

Another area of research is zwitterions. These are useful species in a wide variety of areas including synthesis, chromatography, and the design and construction of novel materials. They are most important in biochemical applications where they are employed as therapeutic agents and make up much of the machinery of life. Specifically, amino acids, proteins, and enzymes exist as dipolar ions over a wide range in pH. The resulting electrostatic field plays a critical role in the structure and function of these molecules. Despite the significance of Coulombic interactions, relatively little is known about their effect on biochemical transformation and the analysis of biomolecules via mass spectrometry.

These researchers have recently undertaken a program to explore the reactivity and thermodynamic properties of dipolar ions in the gas phase. They have carried out extensive calculations on two species, which have helped to interpret photoelectron spectra, to benchmark methodologies, and, most importantly, to gain a better understanding of electrostatic effects. They are now working on amino acid/anion clusters and a host of related systems of biological interest. Because of the number of species that are being examined, the theoretical models that are employed, and the need to explore the molecular conformational space, the resources of the Supercomputing Institute are necessary for this research.

Doreen G. Leopold, Principal Investigator

Computational Studies of Neutral and Anionic NbC_2H_2 Complexes

In this new project, these researchers are using Supercomputing Institute resources to study neutral and anionic transition metal complexes that they have investigated in their laboratory using negative ion photoelectron spectroscopy. The ability to supplement these experiments with computational predictions will aid in the interpretation of these data. Studies will focus on the photoelectron spectrum of NbC_2H_2, with the goal of identifying the isomeric structures and electronic state assignments of the observed anion and neutral molecule states. These results may help elucidate likely mechanisms for the very intriguing reactions that the researchers have observed of ethylene with atomic niobium to form Nb-benzene complexes.

Research Group

Stephen Richard Miller, Graduate Student Researcher

Kenneth R. Leopold, Principal Investigator

Computational Studies of Partially Bound and Hydrogen-Bound Complexes

These researchers used supercomputing resources to carry out high-level quantum chemical calculations on partially bonded and hydrogen-bonded molecular complexes. By providing valuable information about bond energies, molecular structure, and medium effects, the results of these calculations served to enhance the group's ongoing experimental studies.

The main focus of this work is a novel class of molecular complexes for which the researchers have coined the term "partially bound." The distinguishing feature of these systems is that they contain an atom-atom linkage that is neither a weak intermolecular attraction nor a bona fide chemical bond. Thus, the researchers are gaining new insight into the intermediate regime between bonded and non-bonded interactions. Since the presence of a medium has a significant effect on the structures of these systems, the researchers are also studying the effect of a single near-neighbor molecule. They have discovered that microsolvation of partially bound species causes significant changes in structure. Furthermore, the group is investigating molecules that exhibit strong hydrogen bonds in the gas phase, and are also subject to solvent effects. As a whole, the work may be described as fundamental studies of molecular structure and bonding.

The frequencies at which gas phase molecules absorb microwave radiation depend on molecular structure. Since microwave spectroscopy is a high-resolution technique, only a very small portion of the spectral range is sampled per scan, resulting in prolonged spectral searches if molecular structure is not well known. Accurate predictions can, therefore, dramatically reduce spectral search times. Information on bond energies is also of significant interest, and it is not accessible from microwave spectroscopy. Therefore, the researchers are supplementing the experimental results with quantum mechanical calculations that can provide detailed energetic information. They are also applying their calculations to understand the motions within the molecules (e.g., internal rotation and large amplitude vibrations) that may complicate observed spectra.

The final area of research for this group is investigation of medium effects. The researchers have previously demonstrated that partially bonded and some strongly bonded molecules exhibit an extreme sensitivity to the presence of a surrounding medium. They are using microwave spectroscopy to investigate the changes in structure and bonding of such systems that accompany the approach of a small number of near neighbors. Moreover, using existing solvation models, the researchers are using supercomputing resources to allow them to compare the effects of a single molecule with those of an entire medium.

Research Group

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Karin M. Musier-Forsyth, Principal Investigator

Homology Modeling of *Escherichia coli* Proline-tRNA Synthetase and Docking of Modified Proline Analogs

Class II proline transfer ribonucleic acid (tRNA) synthetase (ProRS) catalyzes the specific attachment of proline to cognate tRNA. Although the three-dimensional structure of this enzyme has not been solved yet, the crystal structure of ProRS from a related organism, *Thermus thermophilus*, is known. The active site of the *E. coli* enzyme is quite closely related to the *T. thermophilus* enzyme, and the residues performing analogous functions have been identified by biophysical and biochemical studies.

This research group is elucidating the structure of *E. coli* ProRs based on homology modeling and molecular dynamics simulations, thereby providing a platform for doing docking studies with the cognate substrate proline. This will also allow the researchers to identify *E. coli* ProRS active site residues that are critical for substrate binding.

Research Group and Collaborators

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Computational Chemistry at the Research Site for Educators in Chemistry

The rapid evolution of chemical research away from its traditional core disciplines (e.g., analytical or organic) toward new interdisciplinary disciplines (e.g., computer simulation and modeling or nanomaterials) brings special challenges to four-year colleges. Recognizing that barriers to building sustainable research programs at undergraduate institutions are high, the National Science Foundation (NSF) has created the Research Site for Educators in Chemistry (RSEC) program.

The Department of Chemistry at the University of Minnesota has recently received an NSF grant to establish an RSEC. The focus of this RSEC is four interdisciplinary areas critical to chemistry in the 21st century, including chemical biology, computational chemistry, environmental chemistry, and materials chemistry. The Supercomputing Institute's resources are being used for three areas of research in the computational chemistry field:

- Addressing condensed phase effects of the electronic structure of organic molecules (collaboration with the University of St. Thomas).
- Calculating the absolute free energy of solvation of buyyllithium using a combination of microsolvation and bulk solvation (collaboration with Fisk University).
- Investigating the effects of interfacial adsorption on retention in gas-liquid chromatography (collaboration with Drake University).

Collaborators

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J. Ilja Siepmann, Fellow

Molecular Simulations of Phase Equilibria and Development of Transferable Force Field and Efficient Monte Carlo Algorithms

The Siepmann group's research can be divided into two main areas: simulations of phase equilibria and transferable force fields and efficient Monte Carlo algorithms. There are several on-going projects in these broad areas; some of these are described below.

In the study of phase equilibria, the researchers are studying retention processes in chromatography, structure and solvation in supercritical fluids, structure and solvation in micellar surfactant systems, liquid and solid nucleation from vapor phases, deoxyribonucleic acid (DNA) denaturation and separation, and polymorphism and solvate formation for molecules of pharmaceutical interest. Accurate predictions of phase equilibria and other thermophysical properties of complex chemical systems are of great fundamental and practical importance.

The second broad area of research for this group is developing transferable force fields and efficient Monte Carlo algorithms. The success of molecular simulation in predicting thermophysical properties and in advancing our understanding of the relationship between molecular architecture and macroscopic observables depends on the availability of efficient simulation algorithms and accurate force fields.

One project during this research period investigated adsorption at the gas–liquid interface on retention in gas–liquid chromatography. The importance of this has been controversial for many years; in particular, experimental studies using chromatographic and static techniques to quantify partitioning and adsorption of polar analytes on nonpolar liquid phases yielded conflicting results. In this project, Monte Carlo simulations were carried out for a free-standing liquid slab of squalene surrounded by a helium vapor to investigate interfacial adsorption effect for *n*-pentane, *n*-hexane, *n*-heptane, 1-butanol, and benzene solutes at infinite dilution. The simulations indicate preferential adsorption for the flexible alkane and alcohol solutes in a narrow region just inside the Gibbs dividing surface, but no such effect was observed for the rigid benzene solute. Nevertheless, the extent of the interfacial enrichment is small, as measured by the partition coefficient between the bulk liquid and the interfacial region. In addition, a region that is slightly depleted for all solute molecules was found to separate the interfacial and bulk regions of the squalene slab. Thus, adsorption at the gas–liquid interface should not contribute significantly to the retentive behavior observed in gas–liquid chromatography on nonpolar capillary columns, but might play a role in packed-bed columns with low bonded-phase loadings. The origin for the small enrichments and more favorable free energies for solutes at the interface is that the enthalpies of solvation decrease to a smaller relative extent than the entropies of solvation compared to the bulk liquid.

Another project used coupled-decoupled configurational-bias Monte Carlo simulations in the Gibbs ensemble to determine the vapor–liquid coexistence curve for *n*-tricontane and squalene. The simulations used the transferable potentials for phase equilibria-united atom (TraPPE-UA) force field. The simulated systems consisted of 200 molecules and the production period extended to 100,000 Monte Carlo cycles, a system size about twice as large and a simulation length about one order of magnitude longer than used in previous simulations. The simulation results agree well with the available experimental data. Examination of the coexistence curves in reduced units for the two triacontane isomers and for *n*-octane and 2,5-dimethylhxane shows that both molecular weight and branching can lead to deviations from the principle of corresponding states. Analysis of the molecular structures in the vapor and liquid phases points to a partial collapse (self-solvation) of the triacontane isomers as the likely origin of the deviations from the principle of corresponding states.

In another project, a combination of the aggre-

J. Ilja Siepmann, Fellow

gation-volume-bias and configurational-bias Monte Carlo algorithms and the umbrella sampling technique was applied to investigate two different binary vapor–liquid nucleation systems: water/ethanol and water/*n*-nonane. The simulations are able to reproduce the different non-ideal nucleation behavior observed experimentally for these two systems, i.e., the mutual enhancement of nucleation rates for water/ethanol mixtures and the two-pathway nucleation for water/*n*-nonane mixtures. Structural analysis provided microscopic explanations for the observed nucleation behavior. In particular, the simulations show a large and size-dependent surface enrichment of ethanol in the water/ethanol droplets, which confirms the previous experimental interpretation for this system. The immiscibility observed even for small water/*n*-nonane clusters caused the two-pathway nucleation mechanism.

Research Group and Collaborator

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Donald G. Truhlar, Fellow

Computational Chemical Dynamics

The researchers in this group are studying the structure, dynamics, and thermodynamics of few-body systems, the reaction dynamics of organic, metal-organic, and enzymatic systems, and the influence of solvation of structure and dynamics. A combination of quantum mechanical, quantum statistical, semiclassical, and classical mechanical methods is used to perform the calculations. Some of the Truhlar group's projects are described below.

One area of research is semiclassical and quantum mechanical studies of photochemical dynamics. The group is developing semiclassical trajectory (ST) algorithms for modeling the chemical dynamics of electronically nonadiabatic (non-Born-Oppenheimer) processes. The ST approach is particularly attractive because it approximates the nuclear motion of the system using classical trajectories, and this makes the calculations much more computationally affordable than a full quantum mechanical treatment. The goal of this project is to systematically test these ST methods and to develop more accurate ones as a result of this careful study. The group has developed a method for calculating the adiabatic energies from *ab initio* calculations that does not require any nonlocal information. They have systematically tested and validated several semiclassical trajectory methods including a method called "fewest-switches with time uncertainty," using their set of benchmark systems. They have also developed extremely accurate quantum calculations on the LiFH system at low scattering energies and have observed interesting resonance phenomena, indicating the robustness of their quantum computer code.

In other work, this group has calculated bound-state vibrational energy levels using the VSCF method, and have made progress towards implementing the time-dependent Hartree multiconfigurational self-consistent field method. In another project, Feynman path integrals have been used successfully to calculate free energies for H_2O_2.

Another research area involves applications and development of variational transition state theory (VTST). The researchers are continuing to develop efficient methods for performing thermochemical kinetics calculations. The locally created computer program POLYRATE combines variational transition theory with multidimensional semiclassical tunneling corrections to calculate chemical reaction rates for polyatomic systems in gas- and condensed-phases. One particularly important area of research involves improving the efficiency of electronic structure methods for use with reaction dynamics calculations. The group is continuing to develop hybrid density functional theory and multi-coefficient correlation methods, which have already been shown to perform well for a diverse range of reactions. Recently, the researchers studied the importance of diffuse basis functions when performing density functional theory calculations. The also recently finalized a suite of MCCMs (multi-coefficient correlation methods) called MCCM/3. This set of MCCMs provides an accurate and affordable means of generating potential surfaces for VTST calculations as well as calculating thermochemical properties. They have also performed MC-QCISD and QCISD calculations on the transition states of the direct numerical simulation reaction set. Low-level rate constants for these systems have also been calculated.

The researchers are also investigating enzyme dynamics, and they have successfully calculated kinetic isotope effects for a large number of proton and hydride transfer reactions catalyzed by enzymes. They are continuing to develop the quantum mechanical/molecular mechanical (QM/MM) method with a specific focus on the treatment of the QM/MM boundary region. The generalized hybrid orbital (GHO) treatment of the boundary region has been previously implemented for closed shell systems at the semiempirical level under the neglect diatomic differential overlap approximation framework. More recently, the

Donald G. Truhlar, Fellow

researchers have successfully extended the GHO method to open-shell systems at the semiempirical level. For GHO at the *ab initio* level, a new projection operation has been proposed and implemented to provide a fundamental solution to the non-orthogonality problem. The numerical gradient for the GHO method with the new projection scheme has been implemented, and the fully optimized geometry for a test case showed very promising results.

Another area of research is the reactivity and dynamics of nanoparticles. The focus of this project is the simulation of Al, C, H, and O nanoparticles. The researchers are specifically interested in the nucleation of aluminum nanoparticles and surface reactions with C, H, and O. Critical to the success of this project is the development of new electronic structure methods for aluminum nanoparticles, with accurate calculations for a system that contains more than 100 atoms as the long-term goal. The researchers have performed high-quality calculations on small aluminum clusters, which allowed them to validate less expensive methods that are more suitable for the very demanding calculations on larger nanoparticles. The researchers have found that the methods that are the most favorable are hybrid DFT methods and methods that incorporate pseudopotentials. With the methods applied on small aluminum clusters, the researchers have begun exploratory studies of the energetics of larger aluminum clusters. They have begun to optimize the parameters for tight-binding, pairwise, and three-body potentials for Al.

New charge models have been developed for treating electrostatic effects in boron chemistry and organic chemistry.

Research Group and Collaborators

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Molecular Simulation and Quantum Mechanical Studies of RNA Catalysis

This research group is interested in designing and applying new molecular simulations and quantum models for ribonucleic acid (RNA) catalysis. The particular focus of the project is on four main areas of method development: molecular simulation, hybrid quantum mechanical/molecular mechanical (QM/MM) methods, linear-scaling electronic structure methods, and a new density functional theory (DFT)-based many-body force field. RNA catalysis presents different, and in many respects significantly greater, challenges than do conventional protein systems. The high degree of negative charge, inherently more disordered and dynamical structure, interaction with metal ions, and second row phosphate chemistry all present difficulties that are magnified relative to most proteins. Accurate and efficient quantum models that can treat reactions involving phosphates and monovalent and divalent metal ions are required, as well as methods to adequately sample large regions of configuration space.

The application focus is currently on a prototype RNA enzyme, the hammerhead ribozyme, which is a small RNA motif that undergoes self-cleavage in the presence of Mg^{2+} ions. The researchers are addressing several important structural questions using molecular dynamics simulations in solution and in the crystal, and in the presence of different protonation states and ionic environments. The researchers are studying the reaction using accurate hybrid QM/MM methods with a recently developed semiempirical *d*-orbital specific reaction parameter Hamiltonian. In addition, recently-measured "thio effects" are being studied by replacing the hard Mg^{2+} ions with softer thiophillic Cd^{2+} ions. The researchers have introduced new quantum indices for macromolecular characterization using linear-scaling electronic structure methods applied to the hammerhead ribozyme and to the HIV-1 (human immunodeficiency virus) nucleocapsid protein. Finally, the researchers are addressing basic science issues in the area of solvation methods in DFT and many-body force field development that they hope will have significant impact on future-generation computational models.

Research Group

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Robert J. Dexter, Principal Investigator

Fatigue Strength and Adequacy of Weld Repairs in Ship Structures

Fatigue cracks are not unusual in commercial ships such as tankers and bulk-carriers. These fatigue cracks are primarily an expensive nuisance, requiring weld repairs that often crack again within a short time. A reliable method to estimate the residual fatigue life of typical weld repairs would facilitate rational and efficient design of more reliable weld repairs as well as scheduling for critical inspections.

This project attempts to develop guidelines for specific repairs and to determine the restored life as a result of these repairs. The research involves both experimental work as well as a parametric study using finite element analysis. This analysis is performed using the ABAQUS program on the supercomputers. These parametric studies are compared with experimental results and are used to aid in providing guidelines for optimal repair recommendations.

Research Group

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Clifford Youngberg, Graduate Student Researcher

Robert J. Dexter, Principal Investigator
Carol K. Shield, Co-Principal Investigator

Use of Adhesives to Retrofit Out-of-Plane Distortion-Induced Fatigue Cracks in Multigirder Bridges

During the past 20 years, many multigirder bridges experienced out-of-plane distortion-induced fatigue cracks due to the unwillingness of engineers to weld the connection plane to the tension flange of the girders. Since the connection plate is not positively attached to the tension flange, a gap in the web is produced between the weld at the end of the stiffener and the web-tension flange-weld. The racking motion of the diaphragms produced by the differential deflection of the adjacent girders is accommodated by the short web gap. This can introduce large out-of-plane stress ranges and quickly initiate fatigue cracks within the web gap region. The fatigue cracks are parallel to the in-plane stress field at the initiation phase and will propagate in the direction that is perpendicular to the in-plane stress field. Once the fatigue cracks are perpendicular to the in-plane stress field, the moment capacity of the girder is severely reduced. The distortion-induced fatigue cracks are prevalent in skewed bridges when the staggered diaphragms exist. Increasing the web stiffness by attaching the connection plate to the tension flange of the girders effectively eliminates the out-of-plane problem and is often the preferred retrofit method.

Bolts can be used to attach the connection plate to the tension flange of the girders. However, in the negative moment region, the concrete deck around the retrofit area would have to be removed and traffic would have to be rerouted. An alternative method is to use adhesives to attach a retrofit angle to both the tension flange and the connection plate.

This project consists of three testing phases. First, the researchers made coupon specimens to study the parameters that influence the performance of the adhesives. Then, a field test was conducted to evaluate the performance of adhesives in the field. Lastly, large-scale specimens will be tested to evaluate the effectiveness of the adhesive to decrease out-of-plane distortion under controlled laboratory conditions.

This group is using the finite element program ABAQUS on the supercomputers to complement the laboratory investigation. Analytical models are being constructed to optimize the design of the large-scale specimen. Also, the analytical results will be compared with the test results of both the coupon specimens and the large-scale specimens.

Research Group and Collaborator

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Pre-Stress Cracks in Prestressed Girders; Behavior of an Integral Abutment Bridge

These researchers were involved in two projects using supercomputing resources during this research period. The objective of the first project was to investigate the effect of vertical pre-release cracks on the behavior of prestressed bridge girders. As high-strength concrete becomes more popular, heavily reinforced sections with longer span lengths are being used in prestressed concrete bridge girders. During the production of these girders, it has been observed that vertical cracks near the mid-span of the girders may develop during the curing process if the girders are left on the casting bed for a long time without detensioning the prestressing strands. Cracks have been observed to begin at the top flange and propagate downward in the depth of the section. In some cases they have been observed to extend through the entire depth of the section. The cracking is attributed to restrained shrinkage and thermal effects during the curing period of the girders prior to release of the prestressing strands. Following the release of prestressing strands, the cracks may close completely due to the effects of prestressing force and girder self weight. The cracks were suspected to cause a reduction in the loads required to initiate the flexural cracking in the girder. Analyses done using ABAQUS showed the effects that prerelease cracks have on local girder stresses, flexural cracking load, and girder camber. The second phase of the project includes the experimental validation of the analytical results. The researchers optimized the specimen design and instrumentation using ABAQUS, and performed static and cyclic tests on full-scale prestressed concrete girders. The experimental results verify the analytical study results. The prerelease cracks were found to cause local changes in the beam strains near the crack locations. Even though the effect decayed almost completely away from the crack location, the beams with prerelease cracks had reduced flexural crack initiation loads.

The second project investigates the behavior of integral abutment bridges using the finite-element program ANSYS. An integral abutment bridge is constructed integrally with the abutments, which are designed to allow deformation of the superstructure due to environmental effects. This type of construction, which eliminates expansion joints, results in reduced maintenance costs, as expansion joints are often sources of problems on bridges. An integral abutment bridge was built near Rochester, Minnesota in 1996. Over 150 instruments were installed in and around the bridge during construction to measure the strain, pressure, thermal gradient, settlement, and other behaviors of the bridge. This project's purpose is to develop analytical models to investigate the observed behavior of an integral abutment bridge. A key component of this project focuses on the soil-structure interaction caused by seasonal temperature changes and the integral effect of the whole bridge. The researchers will compare the analytical and experimental results. A finite element model has been established and calibrated by truck loads and temperature loads. In future, parametric analysis will be conducted with different input variables, such as pile types, bridge lengths, soil conditions, temperatures, skewed angles, and so forth.

Research Group

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Bojan Guzina, Associate Fellow

Numerical Solutions in Elastic-Wave Imaging of Subterranean Objects

Elastic (seismic) waves are often used for non-intrusive subsurface sounding for field-testing pavements and geological profiles. Interpretation of the associated surface motion measurements, however, remains a challenge owing to the complexity of the underlying wave propagation phenomena. Based on the traditional uncoupled analyses, the ratio between the material stiffness and mass density is determined from travel times, while the damping characteristics are inferred from the spatial amplitude decay of seismic signals. In cases where the full record of the seismic source is also available, site characterization can be effected more completely in terms of the experimental frequency response functional that relates the applied load to the surface motion in the frequency domain.

Research Group

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Sylvain Nintcheu, Graduate Student Researcher

The goal of this project is to provide an advanced analytical and computational basis for three-dimensional characterization by elastic waves. These researchers are using supercomputing resources to develop a hybrid technique for realistic site characterization that would account for the three-dimensional nature of the induced wave propagation, soil stiffness, density, and damping in a systematic and rigorous manner. It includes the developments in forward and inverse wave propagation analyses and their implementation into an effective field technique for seismic sounding of geological, geotechnical, and pavement profiles. In addition to furnishing independent stiffness, mass density, and attenuation information about the in-site profile that is typically not available from seismic measurements, this method will be capable of an expedient three-dimensional identification of underground objects. A comprehensive delineation of subterranean conditions by means of the proposed technique may be useful for defense applications, construction in urban areas, and pavement monitoring and repair.

Miki Hondzo, Principal Investigator

Computer Modeling of Bubbly Two-phase Flows in Aerated Reservoirs

Aeration is a technique used to improve the water quality of reservoirs that temporarily store combined sewer overflows (CSOs). The U.S. Army Corps of Engineers (USCE) is planning the construction of the McCook Reservoir to store CSOs in Chicago, and the scale of that reservoir is beyond the existing technology of aeration systems. The design will therefore be supported by a combination of laboratory experiments and computational modeling. The development of physically based computer models includes their verification against large-scale experiments and subsequent application to the design of the aeration system for the McCook Reservoir.

This researcher is developing and applying the computer models to simulate flow and water quality that will be used for this project. This analysis will use two computer models, one which already exists and one which is being developed. The existing model, PAR3D, is an ad hoc flow and water quality code developed by Dr. Robert Bernard of the USCE. The new model under development is based on FLUENT, a widely used modeling system used to simulate flow and transport in natural and man-made systems.

Results so far demonstrate that PAR3D predictions agree reasonably well with the mean vertical velocity and turbulent kinetic energy measured in a 25-ft diameter, 30-ft deep tank. Preliminary results obtained using FLUENT 6.0 verify the general pattern and order of magnitude of the PAR3D predictions. A number of different models are being developed using a FLUENT 6.0 mixture model and a Eulerian (fully two-phase) model. Results obtained have been very encouraging.

Research Group

Hong Wang, Supercomputing Institute Research Scholar

Raymond M. Hozalski, Principal Investigator

Modeling Perchloroethene Degradation in Anaerobic Aquifers

Chlorinated solvents are among the most common contaminants detected in groundwater. This is a public health concern because chlorinated solvents are known or suspected carcinogens. These researchers are involved in a large research project investigating the feasibility of promoting *in situ* biodegradation of chlorinated solvents by using gas-permeable membranes to deliver hydrogen to contaminated aquifers.

As a sub-objective of this project, the researchers have developed a complex mathematical model to simulate the transport and microbial transformation of chlorinated solvents and hydrogen in groundwater. The model accounts for the fate of seven solutes (perchloroethene and its four daughter products, plus hydrogen and methane) and also simulates the growth and transport of three microbial populations that compete for hydrogen. One of the microbial populations is undesirable because it rapidly consumes hydrogen, but does not degrade chlorinated solvents.

The mathematical model involves ten interdependent second-order nonlinear parabolic partial differential equations. The governing equations are applied to two adjacent physical domains: an aquifer and a soil-free trench in which the H_2-supply membranes are installed. The domains have different contaminant transport and biotransformation properties and are thus linked by appropriate boundary conditions. A Crank-Nicholson finite differences program has been written in FORTRAN 90 to solve the initial value problem.

Collaborator

Lee Clapp, Department of Environmental Engineering, Texas A&M University–Kingsville, Kingsville, Texas

During this period, these researchers made significant progress with their modeling work. Model simulations predicted that membrane-supplied H_2 could stimulate significant dechlorination rates. However, when the membranes were filled with H_2 at high partial pressures (i.e., greater than ~0.20 atmospheres), meth-anogens utilized most of the supplied H_2. In contrast, when the membranes were supplied with low H_2 partial pressures (i.e., less than 0.05 atmospheres), transfer rates were too low to meet the theoretical H_2 demand associated with a typical perchloroethene concentration of 6 μM. Thus, the model predicted that optimal H_2 partial pressures would be between 0.05 and 0.10 atmospheres.

The model also predicted that biomass would accumulate to very high concentrations within the soil immediately surrounding the H_2-supply membranes and that this would prevent H_2 from dispersing any significant distance. However, although the model did incorporate a maximum biomass threshold to prevent unrealistically high biomass concentrations from accumulating near the membranes, the physical processes of microbial attachment/detachment and advection are not well understood. Comparing the model predictions to experimental results from concurrent soil column studies may improve the researchers' understanding of these processes. The experimental soil column data suggested that the model assumption of no negligible biomass advection was probably realistic, but that the model accuracy could potentially be improved by incorporating homoacetogenesis and acetate utilization by dechlorinators, as well as H_2 production via fermentation of biomass decay products.

Joseph F. Labuz, Associate Fellow
Henryk K. Stolarski, Associate Fellow

Identification of Micromechanisms in Failure of Rock-like Materials

These researchers have used a series of non-intrusive testing methods—electronic speckle pattern interferometry (ESPI) and acoustic emission (AE)—to investigate the failure process of materials such as rock and concrete under wedge indentation. The visualization resources of the Supercomputing Institute are being used to determine the deformation process and estimate fracture parameters from ESPI measurements. Specifically, the fracture toughness of the material is determined from the high-resolution displacements.

Research Group
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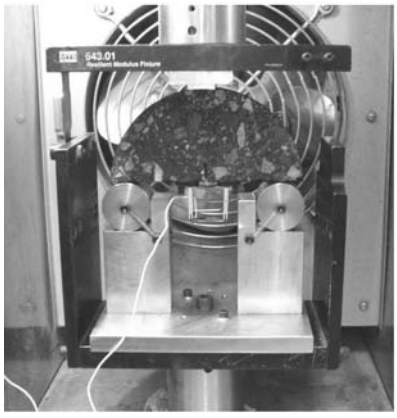
Mihai Marasteanu, Principal Investigator

Low Temperature Cracking of Asphalt Concrete Pavements

Good fracture properties are an essential requirement for asphalt pavements built in the northern part of the U.S. and in Canada, for which the prevailing failure mode is cracking due to low-temperature shrinkage stresses. The current specifications address this issue through the use of strength and creep tests performed on un-notched samples. An increasing number of researchers realize the limitations associated with predicting true fracture properties based on tests performed on un-notched samples. As a consequence, a number of studies have started to investigate the application of the more complex fracture mechanics concepts to the behavior of bituminous materials.

This research group is investigating the use of the semicircular bend test to determine the low temperature fracture properties of asphalt mixtures. The complex geometry of the semi-circular bending specimen makes it hard to find the solution analytically. The researchers are using the finite element method to analyze the stress and strain status numerically. Current results show that a specimen with a thickness of 25 mm can be considered in a plane stress state. The arch effect in both notched and un-notched specimens generates a complex stress condition that makes the explanation of the failure strength measured with this geometry ambiguous.



Semi-Circular Bend Test performed on asphalt mixtures.

Research Group
Xue Li, Graduate Student Researcher

Arturo Schultz, Principal Investigator
Catherine E. French, Co-Principal Investigator

Stability of a Prestressed Concrete Through-Girder Pedestrian Bridge Under Lateral Impact

The objectives of this new research project are to investigate the ductility of prestressed concrete through-girder pedestrian bridges and to investigate the lateral stability of these bridges upon vehicle impact. Prestressed concrete through-girder bridges, in which two prestressed bridge girders support a deck on the bottom flanges, are easy to construct, economical, and durable. Because these bridges are non-redundant, long, simple span structures, vehicle impact could result in collapse if either the girders respond in a non-ductile manner or if the assemblage becomes unstable.

In the first phase of the project, ductility of prestressed concrete girders and the stability of through-girder pedestrian bridge assemblages will be investigated analytically. In parallel, new details including alternate deck and railing systems and/or alternate connection schemes to improve stability will be proposed, if deemed necessary. The second phase of the project will include experimental verification of present and proposed retrofit connection details between the girder-diaphragm and the girder-abutment. Depending on the results obtained at the second phase of the project, a third phase including two large-scale tests of a complete bridge system will be conducted.

Research Group
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Carol K. Shield, Principal Investigator
Jerome F. Hajjar, Associate Fellow

Repair of Fatigued Steel Bridge Girders With Carbon Fiber Strips

Several years ago, it was common that steel cover plates were welded to flanges of hot-rolled steel girders in high moment regions in order to increase the cross section. These cover plates were terminated in negative moment regions, and welds at the ends of cover plates resulted in stress concentrations in the flange. After years in service, these stress concentrations are causing fatigue cracks, and some rehabilitation schemes for these cracks have been proposed.

This project investigates carbon fiber reinforced polymer (CFRP) strips bonded to tension flanges as the rehabilitation method for the fatigued tension flanges. In order to utilize the CFRP strips, it is necessary to find the development length of the adhesive so that the adhesive can transfer sufficient forces from tension flange to the CFRP strips. A series of small-scale experimental tests will be conducted to define the development length, using a stress distribution in the adhesive of the experimental specimens that is similar to that in the rehabilitated girder. The researchers are performing finite element analysis using ABAQUS to enable them to compare the two stress distributions, and to decide which test set-ups can be used. Supercomputing resources are necessary because of the large amount of computation time needed to analyze the stress concentration in adhesive not only due to a singularity in the crack tip, but also because of material non-linearity caused by the high stress concentration.

Research Group
Katsuyoshi Nozaka, Graduate Student Researcher

Henryk K. Stolarski, Associate Fellow
Andrew Drescher, Co-Principal Investigator

Investigation of Factors Related to Surface-Initiated Cracks in Flexible Pavements

Pavement structures (roads) are subject to various adverse conditions, including considerably varying thermal and moisture environments and severe and not-well-controlled loads that are magnified by significant and random dynamic effects. All these conditions occur simultaneously and lead to cracking, rutting, warping, and other signs of road deterioration. At the same time, construction and maintenance of roads is very costly, so there is a need to balance the cost of construction and the cost of maintenance to minimize the overall expenses. That need motivates development of rational tools for design of pavement structures.

This research project addresses one aspect of road deterioration: the mechanism of so-called "surface initiated cracking." In contrast with purely thermal cracking, which typically runs transversely to the road, surface initiated cracking extends longitudinally along the road. This observation contradicts long-held convictions about the nature of various cracks on the roads, which are generally believed to initiate at the bottom of pavements. Furthermore, this cracking is not well understood and is not accounted for in current design procedures. It is likely that an explanation of this relatively new phenomenon would lead to improvements extending the life of the pavement. Given the costs involved, even a small extension of that life would imply significant monetary savings.

The methodology these researchers use is based on the hypothesis that local tire-road interactions may lead to surface tensile stresses which, in comparison with the tensile strength of the material involved, is high enough to initiate surface cracking. The researchers are using ABAQUS to perform numerical simulations to analyze the pavement stress and strain levels in the vicinity of the pavement-tire contact area. The load and geometry of the problem are those found in the most typical practical situations. The researchers are conducting three-dimensional calculations varying parameters such as layout of the road layers and their material properties.

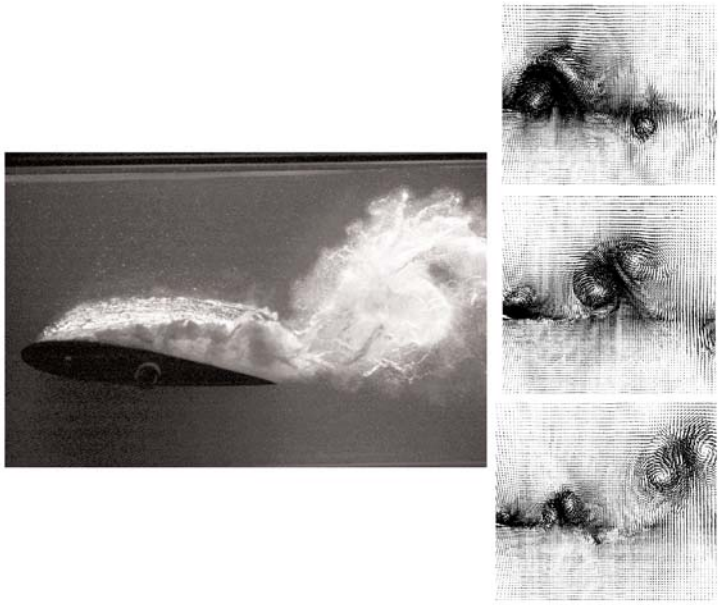
The first phase of this project included two cases, one involving problems with rotational symmetry and the other with plane strain conditions. The main goal of this phase was to determine the extent to which the three-dimensional character of the problem is important. The researchers have determined that, in order to analyze the mechanism of longitudinal cracking in pavements with sufficient accuracy, a three-dimensional analysis is needed. Supercomputing resources are being used to conduct these large-scale, three-dimensional finite element simulations.

Research Group

Jiu Holewinski, Graduate Student Researcher
See-Chew Soon, Graduate Student Researcher

Roger E. A. Arndt, Principal Investigator

Partially and Fully Cavitating Flows



Cavitating flows around hydrofoils fall into three categories: inception (a small number of bubbles near the minimum pressure point), partial cavitation (cavitation extends over less than one chord length), and supercavitation, where the suction side of the foil is fully enveloped in vapor. Partial cavitation has been found to be a highly dynamic form of cavitation. It is responsible for unsteady lift and subsequent shedding of cavitating vortex structures into the wake. A snapshot of this periodic shedding is shown here along with numerical simulations of a vortex pair after being shed from the trailing edge.

Cavitation is an important consideration in a variety of important engineering applications. As the performance of pumps and turbines is increased and hydrofoil ships are designed for higher speeds, it becomes necessary to design lifting surfaces that can operate effectively in the cavitating mode. This group's current research indicates that sheet/cloud cavitation is a highly complex and very important subset of the overall problem. The group has focused on the highly periodic formation of cloud cavitation that leads to a highly structured wake consisting of vortical clouds of bubbles. This phenomenon leads to unsteady lift that cannot be accurately predicted at this stage. This research has now been extended to include fully cavitating and ventilated flows. The goal of the project is to develop the computational tools to study a variety of cavitation problems.

The researchers' interest has been expanded to both numerically simulate and experimentally investigate ventilated cavitating flows. A fully compressible two-phase flow model has been established and the initial results from numerical simulation agree well with those from experiments qualitatively. As cavitation is three-dimensional, the research is being expanded to account for the spanwise effect during the cavitating process. In addition, the researchers are beginning to study the concentration of gas (dissolved and free), which has been shown to have a significant impact on the cavitating wake. They are developing a modified natural cavitating model that accounts for this effect, based upon a barotropic-assumed virtual single phase cavitation model. Using this model, the researchers expect to be able to determine the quantity of gas that comes out of solution during the cavitating process.

Research Group and Collaborator

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Hong Wang, Graduate Student Researcher

Efi Foufoula-Georgiou, Fellow

Multiscale/Multisensor Precipitation Observations for Model Variation and Data Assimilation

Modeling or forecasting of precipitation and other atmospheric and hydrologic variables is necessary for many applications over a wide range of space-time scales. These include flash flood forecasting over small basins, assessment of interseasonal to decadal climate variability at the continental, regional, and basin scale, and assessment of global impacts of climatic anomalies. An obvious concern of all these modeling efforts is the assessment of how well model-predicted precipitation fields compare to the observed fields. However, the observations available for model validation are typically at scales different from the scale (grid size) of the model and comparison is not straightforward.

Another problem that involves comparison or merging of observations at different scales is that of validating satellite estimates of rain. Missions such as the National Aeronautic and Space Administration's Tropical Rainfall Measuring Mission (TRMM) involve numerous ground-based field campaigns and the widespread use of radar and rain gauge networks to validate rainfall estimates from the spaceborne TRMM Microwave Imager, which has a footprint of the order of 20–30 km. A major problem arising when spatial averages of precipitation at one scale are compared or merged with point values or averages at another scale is the fact that the variability of precipitation strongly depends on the scale at which it is considered. How this variability changes with scale is a function of the inherent characteristics of the storm and varies with storm type.

Current methodologies of model variation do not account for the multiscale variability of the underlying process and can result in erroneous or misleading interpretations. The goal of this group's research is to develop a rigorous methodology such that observations or model outputs at different scales can be compared or optimally merged while explicitly accounting for their scale-dependent uncertainties and variability. Such a methodology would result in a minimal representativeness error and the best (in terms of minimum variance) conditional precipitation estimates at any desired scale.

Towards this goal, the researchers have implemented a framework based on the multiscale recursive estimation technique on precipitation measurements from rain gauges (point observations), radars (4x4 km averages), and satellites (16x16 km averages). The scale-recursive estimation procedure consists of two steps, filtering and smoothing. The filtering step uses Kalman filtering, incorporating the measurements of the process and propagating the estimates from fine to coarse scales. The second step consists of smoothing, in which the estimates from the first step are merged with those predicted from the state equation along the coarse-to-fine path. This algorithm has the advantage that it is extremely computationally efficient due to the recursive nature of the fine-to-coarse and coarse-to-fine scale evolutions and the fact that large spatial covariance calculations are not needed. This is especially important with large data sets available at many scales, such as those needed for rainfall, and for real-time data assimilation applications.

Research Group

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Rohit Gupta, Graduate Student Researcher
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Gary Parker, Principal Investigator

Movement of Coarse Sediments in Gravel Bed Streams

The erosion, transport, and deposition of coarse sediments in gravel bed streams constitute the basic processes that define the morphology of a channel bed, and therefore influence the current and potential uses of these streams by people as well as the environmental conditions supporting aquatic life. The estimates of the rates at which these processes happen are commonly based on empirical relationships derived from field and laboratory measurements, and on the understanding of the main physical forces involved. In this regard, a key variable has commonly been the time-average excess bed shear stress or available stream power, variables indirectly computed from direct measurements of flow velocity, water depth, channel bottom slope, bed and bedload particle size distribution, and specific gravity. The accuracy and validity of these measurements for flow and sediment transport modeling calibration are very much influenced by the flow regime and by the sediment characteristics. A different approach is required to handle the uncertainty associated with these mostly assumed time-average values used to calculate the hydraulic response of the channel system, in order to reduce the error in the estimation of the sediment transport process.

The tracking of the displacement of individual bed particles offers an alternative approach that has not been explored with the same enthusiasm as the standard methods, likely because accurate measurements of the relevant variables are more difficult to obtain. Tracer particles have been used for the latter purpose in the past, but a theoretical framework that combines the results of field campaigns and laboratory experiments with an improved knowledge of the stochasticity of the processes and of the effects of the associated time scale has not yet been fully tested. Further, the widely used 30-year-old concept of the active layer (a buffer layer between the sediment moving in the water column and the immobile substrate below) needs to be reviewed to better accommodate the physics of the sediment transport processes. These researchers have recently developed an innovative probabilistic formulation of the problem, but this theory still lacks the development of general predictors for the probability distribution of bed elevation and elevation-specific densities for erosion and deposition of sediment. The researchers plan to perform tracer particle studies in the field and under laboratory-controlled conditions.

The main goals of this research are:

- To identify a relationship between particle displacement distance and bed shear stress over a small time increment and then to integrate that relationship over longer time scales.
- To quantify the bed vertical reworking by floods.
- To implement a numerical model that realistically predicts the morphodynamic time evolution of rivers due to erosion, transport, and deposition of sediment size mixtures.

To this end, the researchers are using supercomputing resources to calibrate and run their numerical model and to process their laboratory data.

Research Group

Miguel Wong, Graduate Student Researcher

Fernando Porté-Agel, Associate Fellow

Large-Eddy Simulation of the Atmospheric Boundary Layer

These researchers use large-eddy simulation (LES) to study the turbulent transport of heat, momentum, water vapor, and pollutants in the atmospheric boundary layer. LES is the state-of-the-art numerical technique to calculate the unsteady three-dimensional transport in turbulent flows. Current limitations in computational resources impose a grid size (~10 m) that is much larger than the smaller scale of motion in the turbulent flow (~1 mm). Until now, LES models have not been sufficiently faithful to the physics of the atmospheric boundary layer. The main limitations of LES are associated with the inability to accurately account for the dynamics that are not explicitly resolved in the simulations.

The main goals of this project are:

- To develop and implement state-of-the-art subgrid-scale models to accurately account for the effect of the non-resolved scales (smaller than the grid size) on the dynamics of the resolved turbulent fields. This is done through the combination of field experiments and extensive numerical simulations.
- To develop improved boundary conditions for the simulations, based on results from wind tunnel experiments as well as numerical experiments.
- To increase the resolution and speed of the simulations by using parallel computing resources at the Supercomputing Institute. The LES code has been modified to run in parallel using message passing interface.
- To generate three-dimensional transient animations of the simulations results.
- To validate the subgrid-scale models being considered based on the field data analysis.
- To visualize eddy structures in the turbulent boundary layer as observed in the field studies.

Research Group and Collaborator

Manual Garcia-Munoz, Undergraduate Student Researcher

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Qiao Qin, Graduate Student Researcher

James R. Stoll, Graduate Student Researcher

Charles C. S. Song, Fellow

Industrial and Environmental Flows

These researchers are developing large-scale flow computation methods and computer codes for scientific and engineering applications, specifically for complex industrial and environmental subsonic turbulent flows. While the Navier-Stokes equations accurately represent real fluid flows of Newtonian fluids such as air and water, complete solution of the Navier-Stokes equations for turbulent flows at large Reynolds number and complex geometry are still not attainable. This group's goal is to advance the state of the art of computational fluid dynamics and to promote its applications to industrial and environmental problems. They will do this by developing improved governing equations and boundary conditions and by developing improved modeling techniques and numerical schemes.

The researchers have developed the compressible boundary layer theory and the computational method based on the weakly compressible flow equations. This approach is about 100 times more efficient than a good conventional method based on the incompressible flow equations. The method can accurately calculate highly time-dependent flows that cannot be computed with the incompressible flow approach.

The group has also developed a computer code for unsteady cavitating flows with and without ventilation. A virtual single-phase approach appears quite successful for natural cavities when there is no ventilation. A two-phase approach is needed when there is ventilation, such as the case when an underwater rocket is under a supercavitating condition. The researchers have developed a fully compressible and weakly compressible code for ventilated supercavitating flow to be applied to an underwater rocket for control purposes. By comparing the results of the two models, the researchers can quantify the effect of compressibility on highly unsteady flows. The existing virtual phase model is being used to further analyze the instability characteristics of sheet and cloud cavity flows over hydrofoils.

These researchers are also developing a new computational model to study the effect of dissolved gas on cavitating flow. Cavitation is known to set dissolved gases free and affect the wake characteristics. The vaporization process is assumed to convert the dissolved gas into a gaseous state in an irreversible manner; once in the gaseous state it permanently remains there. The model is close to completion, and its results will be compared with those from experiments.

Research Group

Xiyangying Chen, Graduate Student Researcher
Qiao Qin, Graduate Student Researcher

Heinz G. Stefan, Associate Fellow

Simulations of Seasonal Water Quality in Freshwater Systems

This research group's on-going objective is to develop and apply computational simulation methods that link hydrology, water quality, and biological habitats in lakes and streams. They have developed deterministic, unsteady, one-dimensional (vertical), year-round lake water quality and fish habitat simulation models. These models have been applied in a continuous mode for many different types of lakes and representing long time periods, including the effects of global climate change. These models are complex, but connect, in a rational way, 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/snow thickness. The lake models have been expanded to take into account the exchange processes between littoral (near-shore) and pelagic (open-water) regions of lakes. The group's current research efforts focus on the effect of rooted aquatic plants (macrophytes) on water quality in the shallow lakes, and models for weekly stream temperature in the continental U.S.

Rooted macrophyte beds in shallow lakes and on the littoral zone of deeper lakes can have a significant impact on both lake ecology and water quality, and are therefore a major component in lake management decisions. As primary producers, macrophytes generate oxygen via photosynthesis, consume oxygen via respiration and decay, and compete with phytoplankton for light. Dense macrophyte beds can modify the water temperature distribution with depth by shading. Macrophytes tend to reduce wind mixing and re-suspension, and increase sedimentation rates. They also play a role in nutrient cycling in lake systems. These effects are manifested directly in shallow lakes and the littoral zone of deep lakes, but may also impact the pelagic zone via advective horizontal transport. While there has been significant research on macrophyte growth and production in lakes, there has been little work to quantify the coupling of macrophytes to lake water quality parameters. The goal of this project is to develop a quantitative understanding of these coupled processes using analytical and numerical process modeling, field measurements, and laboratory experimentation.

The researchers have developed several macrophyte growth models. An analytic growth model has been developed and used to characterize basic macrophyte growth characteristics as a function of both physical and physiological parameters. In particular, the model has been used to analyze macrophyte–phytoplankton competition for light in shallow lakes. A numerical growth model has also been developed to examine more complex scenarios. The numerical growth model serves as the basis for modeling the coupling of macrophyte growth to physical lake processes.

Work is also underway to develop models for the coupling of macrophytes to flow, temperature, and the diffusion of oxygen and other substances. The researchers have developed a model for the influence of aquatic macrophytes on vertical diffusion in lakes. Initial results indicate that dense macrophyte beds dampen wind-generated turbulence very effectively, reducing the thickness of the mixed layer by an order of magnitude. The diffusion model will serve as the basis for the group's

Continued on next page

Research Group

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Sterling Greg Williams, Supercomputing Institute Undergraduate Intern
Jesus Zepeda-Arce, Graduate Student Researcher

Heinz G. Stefan, Associate Fellow

future work on predicting the vertical distribution of temperature, dissolved oxygen, and dissolved inorganic carbon in shallow lakes.

In the second project, the Stefan group is studying the relationship of stream temperature to equilibrium temperature for the continental U.S. Heat exchange between the atmosphere and the water often has a dominant effect on stream temperatures, e.g. by solar radiation and evaporation. However, secondary effects (groundwater, deep reservoir releases, and cooling water inputs) are not always negligible. For approximately 28% of streams in the eastern and central U.S., the heat exchange through the water surface has the most controlling effect on stream temperatures. For the remaining 72%, secondary processes such as groundwater inflow or reservoir releases have an influence. The objective of this project is to apply a full heat budget to a stream reach including terms for the surface heat exchange. Secondary heat sources and sinks such as groundwater inflow, wastewater/cooling water release, and deep reservoir releases are determined by the optimization of model output against extensive multi-year stream temperature data sets for nearly 1,000 gauging stations.

David H. Du, Fellow

Network File System Line Sieving

Researchers have recently developed a new hardware approach to network file system (NFS) line sieving. Current estimates are based on an RSA512 extrapolation and may be too pessimistic.

Collaborator

James P. Hughes, StorageTek, Minneapolis, Minnesota

These researchers are trying to get a more precise picture of factor base sizes that will work for RSA1024. They are developing a program to enable them to find realistic factor base size upper bounds for various reasonable extension degrees. This program is being run on the supercomputers.

George Karypis, Principal Investigator

Scalable Algorithms for Graph Partitioning and Data Mining

This project focuses on developing scalable algorithms for multi-constraint and multi-objective graph partitioning and for mining large scientific datasets. This ongoing research has led to the development of a number of scalable and efficient algorithms.

In the area of data mining, these researchers have developed the first efficient algorithm for discovering frequent sequential patterns whose support decreases as a function of the length of the pattern. This has been an open problem since the early days of data mining research and its solution means that researchers can efficiently find complex patterns that occur relatively infrequently without having to generate an exponential number of simple sequential patterns.

This group has also developed high-quality scalable algorithms for clustering high-dimensional datasets. These algorithms treat clustering as an optimization problem that tries to maximize/minimize a particular clustering criterion function. These algorithms have numerous applications in the areas of information retrieval, micro-array analysis, and commercial datasets. These algorithms have already been made available to the public in the form of a scalable clustering toolkit, called CLUTO, which has been used extensively in a number of application domains and research projects.

Research Group
Irene Moulitsas, Graduate Student Researcher

Youngdae Kim, Principal Investigator

Secure Group Communication

Secure group communication has received much attention in recent years. Since most group communication takes place over the Internet, security is a major concern. The fundamental security challenge revolves around secure and efficient group key management. Centralized key management methods (key distribution) are appropriate for two-party (e.g., client-server or peer-to-peer) communication as well as for large multicast groups. However, most collaborative group settings require distributed key management techniques.

This research project studies all security aspects of peer groups. Security problems in peer groups are challenging and interesting due to their distributed and non-hierarchical nature. Each group member has the same rights and no trusted parties are assumed. Every decision and action (ideally) should be decided collaboratively. Examples of peer groups include group communication systems, peer-to-peer systems such as file sharing and content distribution, MANETs (Mobile Ad Hoc Networks), and anonymous communication systems. Security issues in such environments can be enumerated as: key management, signature mechanisms, public key infrastructures, admission control protocols, and security policy negotiations. These researchers are attempting to provide solutions to these issues in conjunction with different communication systems.

Research Group
Vishal Kher, Graduate Student Researcher

Vipin Kumar, Fellow

High-Performance Data Mining for Cyber Threat Detection

Our nation depends critically on the information infrastructure to maintain economic and military leadership in the world. The emerging networked society is increasing this dependence, making us more vulnerable to attacks against the infrastructure. The overall objective of this research is to develop high performance data mining algorithms and tools that will provide support required to analyze the massive datasets generated by various processes that monitor computing and information systems. This research is being conducted as a part of the Minnesota Intrusion Detection System (MINDS) project that is developing a suite of data mining techniques to automatically detect attacks against computer networks and systems.

Research Group and Collaborators

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The University of Minnesota network security analysts have been using MINDS to successfully detect novel intrusions that could not be identified using state-of-the-art signature-based tools such as SNORT. Many of the attacks detected by MINDS have been reported on the CERT® Coordination Center list of recent advisories and incident notes. Although the techniques developed to date are very promising, they are preliminary in nature and they do not scale to very large network traffic datasets. High-performance data mining algorithms can address large datasets, but developing these algorithms for network intrusion analysis is challenging for many reasons. For example, many association rule analysis algorithms require that all the data need to be resident in main memory, which is clearly untenable due to the large size of the network data. In addition, cyber attacks may be launched from several different locations and targeted to many different destinations, thus creating a need to analyze network data from several networks in order to detect these distributed attacks. Therefore, development of new distributed anomaly detection algorithms that can take advantage of high performance computers and be computationally tractable is a key component of this project.

Gary W. Meyer, Principal Investigator

Level-of-Detail Systems

Level-of-detail (LOD) systems are used to simplify highly complex three-dimensional models. These models are often too high-resolution to render on personal computers at interactive rates, so an LOD system will attempt to reduce the complexity of the model to allow for interactive rendering. Historically, LOD systems use simple geometric error estimates to determine when and where to reduce the complexity of the model. This can lead to unusual artifacts and changes to the model that are easily visible.

A visual difference metric (VDM) is a model of the human visual system that attempts to locate and measure the differences between two images that a human user would see. It takes into account things such as light intensity, sampling by the human eye, and contrast changes to determine how much difference there is between the two images from a human perspective.

These researchers are using a VDM on an LOD system also in development to create mapping between the parameters of the LOD system and the desired human visual similarity of the finest resolution model to the LOD-simplified model. This should give more accurate and visually appealing results than a simple geometric measurement. The results from this research may potentially be applied to many other LOD systems, resulting in high-LOD systems that display visually accurate models at interactive frame rates.

Research Group

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Haesun Park, Principal Investigator

Data Space Dimensional Reduction for Support Vector Machines

These researchers are investigating sampling methods for data mining. Three methods have been used and compared: the support vector machine (SVM), the Nyström method (instance based algorithm or IB2), and random sampling. The random sampling strategy was the best in terms of model independence, but its random nature can sometimes result in a catastrophic lack of accuracy. SVMs performed the worst overall, although this method minimized structural risk. The researchers are continuing this study to try to find a better selection method.

A new project for this group involves the prediction of disulfide bonding states. The researchers will study the prediction of disulfide connectivity by using the machine learning approach to consider the environments of two binding cysteins.

Research Group

Shyam Boriah, Graduate Student Researcher
Hyunsoo Kim, Graduate Student Researcher
Cheong Hee Park, Graduate Student Researcher

Yousef Saad, Fellow

Parallel Algebraic Recursive Multilevel Solvers

In the last few years, this research team has developed a package for parallel sparse matrix computations called pARMS (parallel Algebraic Recursive Multilevel Solver). The aim of this package is to provide a collection of iterative techniques for solving large, sparse, irregularly structured, linear systems of equations on parallel platforms. The package includes all the preconditioning techniques available in its predecessor (PSPARSLIB) as well as a new class of methods that are based on recursive algebraic multilevel techniques.

Research Group and Collaborators

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Na Li, Graduate Student Researcher
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Laurent Smoch, Research Associate
Masha Sosonkina, Faculty Collaborator
Azzeddine Soulaimani, University of Montreal, Montreal, Quebec, Canada

Recent work on this package includes intensive research focused on improving the performance of parallel iterative solution methods from the pARMS library. Supercomputing Institute resources were the main testing and implementation platforms for this effort.

The researchers have also continued work on the Schur Complement preconditioning and have studied the performed of the preconditioning on the subdomains with overlapping. Other, more sophisticated preconditioners for the Schur Complement system have also been devised.

Finally, reducing the parallel overhead has enhanced parallel efficiency of a parallel iterative solver. For a Block-Jacobi preconditioning, the "fast" processors were allowed to perform more iterations instead of idling while waiting for slower ones.

Stephen A. Campbell, Principal Investigator

Nanoparticle Device Research

These researchers are attempting to build transistors and other semiconductor devices using single crystal silicon nanoparticles. As integrated circuits are scaled down, speed is increasingly limited by interconnect effects. A radical way to reduce this problem involves replacing the single crystal silicon wafer with small, crystalline silicon particles. This would allow building many layers of transistors and interconnect layers on arbitrary substrates. Since the particles are created in the gas phase, they can be annealed at very high temperatures, thus removing impurities and extended defects. They can then be captured on a substrate and used to make devices. Such an architecture would allow the formation of devices containing any type of device (transistors, lasers, diodes, radio-frequency components, magnetic memory) on any type of substrate (plastics, mylar, glass). Ultimately this would move information technology out of metal boxes and into clothes, contact lenses, and other low-cost consumer items.

This vision hinges on the ability to form single crystal silicon spheres in the gas phase, process the silicon, and localize those spheres on a substrate. In the first part of this project, the researchers are modeling their reactor, which creates the silicon nanoparticles. They will design an aerodynamic lens, a system that allows them to strip the particles they create from the reactive gases in which they were formed. This is a necessary first step to annealing, processing, and localizing the particles. This work uses the computational fluid dynamics program CFD-ACE to predict the gas streamlines in the reactor.

Research Group

Ying Dong, Graduate Student Researcher
Bek Ligman, Graduate Student Researcher

Anand Gopinath, Associate Fellow

Modeling of Vertical Cavity Lasers

This research group developed a self-consistent model of the Vertical Cavity Surface Emitting Laser (VCSEL), 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 thus expensive cleaving of the crystals and alignment of the facets normal to cleave planes are avoided. The disadvantage of these devices is that devices with diameters of the order of 10 μm and larger quickly become multimode, and thus the spectrum of emission has many lines. The goal of this project is to find a means of keeping these devices in single mode for all diameter sizes. The researchers are doing this by building a detailed model of the VCSEL.

The researchers have written a scalar two-dimensional code for the cylindrical geometry in terms of *r-z* coordinates, and all the modes possible for the transverse electric (TE) and transverse magnetic (TM) modes have been identified and categorized. The researchers are now writing the vector code in the cylindrical *r-z* geometry with rotational symmetry to calculate the hybrid modes of the structure.

A new area of research for this group is the modeling of photonic band gap media and methods of placing optical waveguides in it. The structures being investigated are the colloidal opal and the inverse opal structures. The researchers are modeling these structures and have completed some preliminary work.

Research Group

Kung-Hyun Baek, Graduate Student Researcher
Chanin Laliew, Graduate Student Researcher
Ross Schermer, Graduate Student Researcher

James E. Holte, Principal Investigator

Tracing Fluids Through Human Airways

This research group is studying the movement of mucus in the human airways in order to find better treatments for cystic fibrosis. Since the development of the symmetrical bronchial tree model of the lung, many researchers have sought to revise this model. This project will establish a model for the bronchial branches of the human lung and analyze the airflow caused by inspiration and expiration. The limitation of computer power does not allow for modeling the whole bronchial system, nor does it allow for analysis of airflow from the upper airway to the deepest branch simultaneously. Instead of developing one large model, these researchers are visualizing the bronchial branches as numerous building blocks. The airflow within each block will be calculated separately.

This model will be used to simulate the high-frequency chest compression method of eliminating mucus in the human airways as a treatment for the symptoms of cystic fibrosis. This will help researchers find the best treatment for treating patients with this disease.

Research Group and Collaborator

Kiwon Sohn, Graduate Student Researcher
Warren J. Warwick, Faculty Collaborator

James R. Leger, Associate Fellow

Electrical-Magnetic Field Simulation for Micro-Optical Elements

This project investigates the properties of micro-optical elements. Information about the electromagnetic fields inside and outside of micro-optical elements is crucial and needs to be studied numerically. These researchers have applied the rigorous-coupled-wave (RCW) method to simulate two-dimensional periodic micro-optical elements and have achieved good results. Their mass transport technology enables them to fabricate various micro-optical elements so that they can compare their computer model with experimental results. Given sufficient computational resources, the current model can handle many realistic structures. However, to simulate more complex structures, a three-dimensional non-periodic model is necessary. The next goals of the project are to improve the current model and to develop a three-dimensional model. The results will be compared with experimental measurements.

During the past year, the researchers were able to study the near field phenomena. Based on the simulation, they found that it may be possible to measure the refraction indices of very thin film with much better accuracy than the current technique. The researchers also performed studies based on the RCW method to investigate the polarization effects from sub-wavelength structures. The results of the simulation agreed well with experimental data. This method has also been applied to the study of photonics crystals.

Research Group

Zhaohui Zang, Graduate Student Researcher
Qiwen Zhan, Graduate Student Researcher

David J. Lilja, Fellow

Execution-Driven Simulations of Future Computer Architectures

This research group's focus is to exploit the interaction of compilation technology and parallel computer architecture to improve the performance of future processor architectures. The group is working on several projects that fall under this broad goal. Descriptions of some of these projects appear below.

One project seeks to characterize the spatial behavior of static and dynamic load instructions. So far, the researchers have examined the following characteristics:

- The distribution of where loads get their value in the memory hierarchy (i.e., caches of memory).
- The number of memory misses due to the most problematic static and dynamic loads.
- The properties of those problematic loads.
- The number of effective addresses referenced per static load and the number of static loads that reference each effective address.
- The invariability of the previous four characteristics for different program inputs.

Research Group

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A. J. Klein-Osowski, Graduate Student Researcher
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Keqiang Wu, Graduate Student Researcher
Joshua J. Yi, Graduate Student Researcher

Eventually, this project will examine the temporal characteristics of static and dynamic load instructions, in addition to trying to create dynamic (vs. static) methods of performing this characterization.

In another project, the researchers are investigating the effect of executing mispredicted load instructions. The researchers have proposed a new technique, which is based on the wrong-path execution of loads far beyond the instruction fetch-limiting conditional branches, to exploit more instruction-level parallelism by reducing the impact of memory delays. They are examining the effects of execution of loads down the wrong path on the performance of high issue-width processors. They proposed the wrong-path cache to reduce the pollution caused by the execution of loads down mispredicted paths. This project is being extended to include a speculative multithreaded architecture.

The researchers are also investigating the performance potential of dynamically eliminating repetitive computations by using profiling to identify highly redundant computations. The researchers are refining the current implementation, incorporating new features, and more fully exploring the design space.

The researchers are developing a new technique, address correlation, to improve data cache performance. A store instruction can store the same data value to more than one memory location. Furthermore, recent research has introduced the concept of frequent value locality, in which a few values appear very frequently in memory locations and are therefore involved in a large fraction of memory addresses. By using these two observations, the researchers are using the new address correlation technique to link the addresses that reference the same (frequent) data. Preliminary results show that there is substantial potential to hide the memory latency by using the data from a correlated address instead of the requested address,

David J. Lilja, Fellow

thereby converting a cache miss into a cache hit. The correlation of addresses may also introduce new techniques for aligning the cache coherence protocols in multiprocessor systems.

Another project investigates cache scaling for accurate performance simulation. To reduce the time required to simulate complete processor designs, one reduces the inputs to the benchmark program that drives the simulation. However, one potential side effect of this reduction is that the L1 cache miss rates are not truly representative of what they are when using the reference inputs on a real system. Therefore, to produce accurate simulated miss rates, the goal of this project is to determine scaling factors for the key cache parameters.

Ned Mohan, Principal Investigator

Investigation of Non-linear Mutual Coupling in Switched Reluctance Machines

Switched reluctance machines (SRMs) have been gaining acceptance due to their inexpensive and robust construction and the fault-tolerant electronics used to operate them. Traditionally, a per-phase model of an SRM is used for predicting dynamic operation and developing control strategies. This model does not account for the fact that all SRMs operate with more than one phase energized at all times.

The objective of this project is to formulate a model that accounts for these non-linear interphase couplings. Such a model would lead to improved accuracy in the prediction of phase currents and electromagnetic torque, leading to controls that will optimize efficiency and torque pulsations. It will also allow more accuracy in the prediction of mutually induced voltages in unexcited phases that can be used for designing position sensing schemes. This requires accurate electromagnetic characterization of the motor.

These researchers are using Supercomputing Institute resources to conduct a finite element analysis, which will be correlated with experimental results.

Research Group

Todd Begalke, Graduate Student Researcher
Amit Kumar Jain, Graduate Student Researcher

P. Paul Ruden, Associate Fellow

Properties of Semiconductor Materials and Devices

The goal of this ongoing research is to advance the understanding of novel semiconductor materials and devices. The most recent work has concentrated on electronic devices made from large band gap semiconductors, specifically III-nitride compounds and organic semiconductors.

The electronic properties of semiconductor devices are strongly influenced by built-in or externally applied stresses. For the III-nitride materials in particular, stress effects are of critical importance due to their strong piezoelectric properties. The bandstructure of holes in a p-structure AlGaN/GaN heterostructure is very sensitive to applied stress. These researchers have recently developed codes that allow for a first-order quantitative assessment of these electronic structure effects that are also beginning to be explored experimentally.

The AlGaN/GaN heterostructure calculations involve the self-consistent solution of coupled Schroedinger and Poisson equations. The Schroedinger equation consists of six coupled differential equations describing the III-nitride valence bands of interest. These equations must be solved separately for different k-points. The researchers have implemented a scheme of parallel computation of multiple k-point solutions to achieve convergence within a reasonably short run time.

This group has started a new project to model organic field effect transistors (OFETs). The initial focus was on the formation of a conducting channel, and current work is directed towards an examination of the direct current device performance. Recently, the researchers obtained results for the output characteristics and the surface potential of OFETs. Current work focuses on calculations needed for the interpretation of experimental data, particularly surface potential data.

Research Group and Collaborator

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Dominic Schroepfer, Graduate Student Researcher

Nikolaos D. Sidiropoulos, Principal Investigator

Tri- and Multilinear Methods for Signal Processing and Communication Engineering

This group is conducting research on tri- and multilinear methods in signal processing for communications engineering. The starting point is the trilinear model, also known as trilinear decomposition or Parallel Factor (PARAFAC) analysis. It was first introduced as a data analysis tool in psychometrics, and has also been used in phonetics, exploratory data analysis, statistics, arithmetic complexity, and other fields and disciplines. It is mostly used now in the context of chemometrics, where it is used for spectrophotometric, chromatographics, and flow injection analyses. In signal processing and communications terms, PARAFAC can be thought of as a generalization of Estimation of Signal Parameters via Rotational Invariance Techniques (ESPRIT) ideas—actually as a general principal underlying the most general formulation of ESPRIT to date. PARAFAC can also be seen as generalizing joint approximate diagonalization ideas.

This group looked at applications of PARAFAC in sensor array processing, wireless multisensor communications, wireless packet radio networks, and source separation. They have also contributed to the theory of multi-way analysis, particularly toward uniqueness/identifiability results. They are developing efficiently fitting algorithms for the PARAFAC model and derivatives/generalizations.

Research Group

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J. Thomas Vaughan, Principal Investigator

Simulation of High Frequency RF Volume Coils in Magnetic Resonance Imaging

Radio frequency (RF) coils play a key role in magnetic resonance imaging by generating RF pulses at the Larmor frequency to excite the nuclei in the objects to be imaged and by receiving the signals from the objects at the same frequency. However, as the frequency increases, radiation losses rise dramatically and become important, which affects the efficiency of the coils and causes the image quality to deteriorate. These researchers are simulating and studying this effect using the resources of the Basic Sciences Computing Laboratory.

Research Group

Jinfeng Tian, Graduate Student Researcher

Randall H. Victora, Associate Fellow

Micromagnetic Simulations of Head and Media for High-Density Magnetic Recording

Magnetic recording technology has been extensively developed for application to information storage devices such as computer hard disk drives. Recording density has significantly increased every year with the growing application of sound and image data that demands very large storage capacity. Average hard disk drive capacity has been increasing annually by 1.6–2 times. Thermal decay, however, which makes recorded information unstable or ultimately causes loss of information, has been a technical barrier in the development of higher-density technology. The density limit imposed by thermal decay in existing longitudinal recording media has been estimated at 100 Gb/inch^2. To surpass this limitation, new magnetic recording materials must be developed. Magnetic thin films with perpendicular uniaxial anisotropy have been experimentally studied for this purpose.

These researchers have developed a numerical model that uses micromagnetic theory to simulate the magnetic characteristics of perpendicular recording media. A realistic grain configuration (planar Voroni cells) is used to represent the thin film media. In this micromagnetic model, the total energy of the studied piece of material is expressed as a function of the angles of magnetization (independent variables). The model takes into account not only the crystalline anisotropy energy and the self-demagnetization energy, but also the magnetostatic interaction energy and the quantum exchange coupling energy between grains in the total system energy. The researchers have also made provisions for the incoherent rotation of the magnetization within a grain. This adds complexity to the calculation owing to the need for multiple nodes within one grain. The exchange coupling energy is assumed to be proportional to the area between two grains. The magnetostatic interaction field between two grains is calculated by using a geometric mapping technique. The total effective field within a grain is obtained by differentiating the energy with respect to magnetization. The equilibrium of the whole film system is achieved by locally minimizing the energy of each grain. This dynamic procedure is governed by the non-linear Landau-Lifshitz-Gilbert differential equation, which is integrated iteratively.

This group's most significant result has been their discovery of a recording head design suitable for a density of 1 Tbit/inch^2. The problem with recording heads at such high density is the difficulty in channeling the flux down to the soft underlayer through the recording media despite the small track width (50 nm) and large spacing (30 nm). Using an unusual stepped head design, these researchers were able to approximately double the expected value of the head field to 15 kOe while maintaining excellent field gradients exceeding 300 Oe/nm. Supercomputing resources were used not only to obtain the original design, but also to test the new head for features such as switching time and media stability. Subsequent work has explored the parameters of this design, particularly the extent to which the magnetization and anisotropy of the recording layer can be reduced and still be thermally stable. As part of this effort, the researchers have used the supercomputers to find a general expression for the scaled temperature in their micromagnetic stability calculations and as a function of grain size, anisotropy field, and magnetization. They have also simulated writing on these new materials. The major results are that the anisotropy field can be reduced from 20 kOe to 17 kOe or the grain magnetization can be reduced from 800 emu/cm^3 to 600 emu/cm^3.

Research Group

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JianhuaXue, Graduate Student Researcher
Enhong Yuan, Graduate Student Researcher

Randall H. Victora, Associate Fellow

This should increase overwrite performance and reduce neighborhood induced transition shift, respectively.

Another achievement by this group is the successful prediction of the hysteresis loop in a material for which switching occurs by domain nucleation and propagation, as opposed to coherent rotation where accurate predictions have become commonplace. In particular, they calculated that, for Co/Pt superlattices, domain nucleation occurs many times per second at the sharp-cornered grain boundaries within the Co layer. Although most times these domains are rapidly extinguished by the exchange interaction from the neighboring material, the researchers showed that occasionally they can grow and propagate through the crystal.

Babak Ziaie, Principal Investigator

Integrated Inductor Quality Factor Degradation in Tissue

Many implantable wireless microsystems (passive and active) use integrated inductors for power transmission and signaling. A high quality factor coil improves the power transmission efficiency and signal-to-noise ratio. However, the effect of tissue proximity on the quality factor of these coils is not adequately investigated. These researchers are using experimental and computation methods to measure and model the effect of various tissues (e.g., muscle, fat, and skin) in quality factor degradation of integrated inductors. Initial measurements in muscle tissue have indicated a 50% decrease in the quality factor. The researchers are now using the Scientific Development and Visualization Laboratory to perform electromagnetic simulations on multi-turn integrated inductors embedded in various tissues. This will increase their understanding of different sources of loss and its dependence on tissue properties such as resistivity, anisotropicity, and dielectric constant. This will also allow the researchers to optimize the inductor design and implantation technique in order to prevent significant quality degradation.

Research Group

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William E. Seyfried, Principal Investigator

The Solubility of Quartz in the Low-Pressure Supercritical Region of Seawater

Mineral solubility at elevated temperatures and pressures provides the primary means for mass transfer in sub-seafloor hydrothermal systems at mid-ocean ridges. These hydrothermal systems are the largest on the earth and are primarily responsible for maintaining the composition of seawater at steady state values throughout geologic time. Although there have been numerous experiments measuring the solubility of minerals such as quartz at a wide range of temperatures and pressures, data do not exist at the critical point of seawater where hydrothermal conditions tend to occur most often. For this reason, new experiments at this pressure-temperature region are required.

These researchers are using the Basic Sciences Computing Laboratory to perform molecular dynamics calculations that will allow them to better understand the conceptual framework for experimental data. The combination of experimental and theoretical constraints will go a long way toward understanding phase relations involving quartz in sub-seafloor hydrothermal systems.

Research Group

Dionysios I. Foustoukos, Graduate Student Researcher

David A. Yuen, Fellow

Numerical Modeling and Visualization of Geophysical Processes

The Yuen group's research is focused directly toward a quantitative understanding of the earth's interior from numerical modeling of complex physical-chemical and fluid-dynamical processes. They are actively engaging in scientific visualization, also called "visual computing."

The topics of this research include:

- Large-scale computations of three-dimensional thermal convection with focus on both basic fluid dynamics and geophysical applications, such as the incorporation of phase changes, viscous dissipation, adiabatic heating, and strongly temperature-dependent and non-Newtonian viscosity and temperature- and pressure-dependent thermal conductivity associated with silicate rocks inside the earth's mantle.
- Numerical simulations of two-dimensional convection problems with both complex physics and chemistry, such as grain-size dependent rheology and plastic yield strength, variable thermal conductivity and complicated geological boundary conditions, as applied to basic questions in fluid mechanics and applications in the evolution of planetary interiors. This includes finite element modeling of the thermomechanical evolution of the continental lithosphere and subduction processes.
- Large-scale mixing by convective flows, shear flows with different types of microscopic mesoscopic and rheologies present, and viscoelastic calculations by an adaptive wavelet transform technique and multifractal analysis studies of chemical mixing processes involving contaminated chemicals and their reactants in nuclear waste tanks.
- Large-scale regional visualization of seismic

David A. Yuen, Fellow

wave data and the inference of actual three-dimensional structures in the upper mantle by continuous Gaussian wavelet transforms and scientific visualization of the phase gradients obtained in radar interferometric images from satellites.

- Large-scale molecular dynamics simulations of micro-hydrodynamical phenomena in the range of 100 angstroms and thin-film problems with dissipative particle dynamics.
- Three-dimensional convection in a spherical-shell model using a spectral finite volume technique with an extremely high resolution of 1/3 to 1/5 degrees.
- Mapping seismic mantle probabilities with the Neighborhood Algorithm. The composition and dynamics of the earth's deep mantle can only be understood if robust seismic constraints on the three-dimensional patterns of mantle density and velocity are combined with constraints from mineral physics and geodynamics. Free oscillation and surface wave seismic data below 10 mHz provide enough resolution of the deep mantle to retrieve robust constraints on structure, but the large null space of this inverse problem implies that these constraints must be described with probabilities, rather than with individual best-fit models. To retrieve model probabilities, one must first examine the fit to the data achieved by large and representative sets of possible models. The researchers are using the Neighborhood Algorithm to do this, as it is more easily implemented than genetic algorithms.

Research Group and Collaborators

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Dennis A. Hejhal, Fellow

Computational Aspects of Analytic Number Theory

This research group continued its computational analyses of high frequency eigenfunctions of the Laplacian on fuchsian groups. Jobs were run in Sweden on a Cray YMP-EL and Cray-T3E. Codes derived from work performed at the University of Minnesota play a vital role in the analysis. The group has recently calculated the value distribution as well as local moments of "CM-forms," a special kind of eigenfunction of the Laplacian. The aim here was to determine if any statistical anomalies would be visible when passing from a generic to "almost deterministic" setting. The group is also considering statistical properties of automorphic forms on a variety of non-arithmetic arithmetic fuchsian groups. In the case of CM-forms, results supporting a general correlation conjecture of M. V. Berry have been obtained. The group plans to explore CM-forms further in certain higher-dimensional settings.

Collaborators

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John S. Lowengrub, Fellow

Topological Transitions and Singularities in Fluid, Crystal, and Biological Interfaces

These researchers are continuing their study of topological transitions and singularities of interfaces in fluid flows and biological systems, using their dual approach of sharp and diffuse interface methods. In fluid systems, the group is continuing to investigate interfacial flows with and without surfactants and flows in which the components have varying miscibility. They also perform high-resolution simulations of droplet coalescence and break-up. In crystals, the researchers study the evolution of three-dimensional crystals with isotropic and anisotropic surface tension and kinetics. In biological systems, they are continuing their work on the morphology of non-necrotic vascular tumors.

The goals of the fluid dynamics aspect of this research are:

- To investigate interfacial flows with and without surfactants using accurate, spatially adaptive sharp interface methods.
- To refine and validate a physically based method to capture pinch-off and reconnection in liquid/liquid interfacial flows.
- To develop diffuse interface methods to simulate visco-elastic flows.

To this end, the researchers have developed efficient and accurate sharp-interface methods in which to simulate interfacial motion in three-dimensional viscous flows. This approach uses a finite element method. The interface is represented using a triangulated surface and the volumes in the interior and exterior of the interfacial surfaces are discretized using tetrahedra such that the triangulated surface is the boundary of the volume tetrahedra. A critical component of this work is the use of adaptive, unstructured surface and volume meshes. The surface adaptivity is performed using the algorithm developed by Cristini et al., and the

John S. Lowengrub, Fellow

volume tetrahedra are constructed from the surface triangulation using an advancing front algorithm (using the HYPERMESH software package). The researchers have used this algorithm primarily to simulate the motion of viscous drops in Stokes flows. However, the algorithm is much more general and the researchers have begun using it to investigate visco-elastic interfacial flows.

In another project in this area, these researchers have developed a diffuse interface model that overcomes the difficulty encountered with the sharp interface model historically used to represent the narrow zone separating immiscible fluids. The latter model breaks down and singularities form when interfaces pinch-off and reconnect. Further, in this model, one has to prescribe ad hoc "cut-and-connect" conditions to evolve the flow through these events. In the new model, 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. The researchers have used this partial miscibility model (PMM) to solve several flow regimes. They have also studied the pinch-off of thin viscous threads of fluid, and have extended the PMM to the case of ternary fluid flows.

In recent work in the area of crystal growth, the researchers are studying the three-dimensional morphology of growing solid crystals in a liquid melt as well as the growth of precipitates in solid-solid phase transformations. This involves solving a diffusionally evolving free boundary problem. The linear analysis suggests that, under certain conditions, the morphology of growing crystals may be controlled. The group has confirmed this with numerical experiments. They have recently developed a fully adaptive, three-dimensional boundary integral method to solve the diffusional evolution of interfaces. They are beginning with isotropic surface tension, and have begun to extend their results to anisotropic interface kinetics.

The group's research on tumor growth focuses on the tumors' stability. It is important to know under what conditions tumors tend to break up, since this increases the danger of cancerous cells spreading throughout the body. The researchers are developing level-set based methods capable of handling topological transitions, a necrotic core, and tumor angiogenesis (the development of blood vessels from the main vasculature to the tumor).

Research Group and Collaborators

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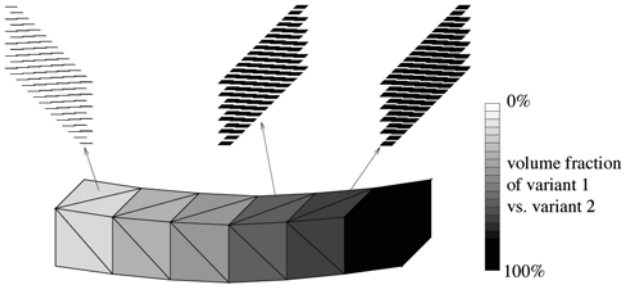
Computation of Active Martensitic Thin Films



Microstructure for cubic to orthorhombic martensitic phase transformation computed with piecewise laminates (Krusik and Luskin).

These researchers are 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 goal of this project is to develop the ability to simulate the behavior of shape memory materials, most of which undergo a martensitic transformation. The researchers are developing a computational model that can simulate the experiments being performed in the James laboratory on a Cu-Al-Ni shape memory alloy.

Research Group

Giuseppe Fadda, Supercomputing Institute Research Scholar

Energy-minimizing sequences of deformations for martensitic crystals modeled by the Ericksen-James elastic energy density often exhibit a microstructure—the simplest of which contains layers in which the deformation gradient is nearly constant and across which the deformation gradient oscillates between energy wells—to 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, these researchers have developed computational methods to approximate microstructure and a mathematical theory that has made possible rigorous analysis of numerical approximation of microstructure.

Hans G. Othmer, Fellow

Mathematical Modeling of Vertebrate Limb Development

This research project expands a previously developed, two-dimensional model for limb development. The model incorporates outgrowth due to cell growth and division, as well as interactions between morphogens produced in the zone of polarizing activity and the apical epidermal ridge. The numerically computed, spatio-temporal distributions of these morphogens demonstrated the importance of interaction between the organizing regions in establishing the morphogenetic terrain on which cells reside. The researchers also found that, because growth is explicitly incorporated, the history of a cell's exposure to the morphogens depends heavily on where the cell originates in the early limb bud. The mathematical model and the associated computational algorithms were sufficiently flexible that other schemes for the interactions between morphogens, and their effect on the spatio-temporal pattern of growth and gene expression, could easily be tested. Thus an additional result of these researchers' previous work is a computational tool that can be used to explore the effects of various mutations and experimental interventions on the growth of the limb and the pattern of gene expression.

During this period, the researchers used Supercomputing Institute resources to simulate the effect of surgical interventions during the limb formation process on the spatio-temporal morphogen distribution. This model was successful in explaining recent experimental results that had appeared to be counter-intuitive. Because the present model is in two dimensions, it does not take into account dorsal-ventral polarity. The researchers have now constructed a three-dimensional framework of molecular interactions that will enable them to generate a complete and more accurate picture of the events during limb formation. This will be the basis of the "reaction" part of the three-dimensional reaction-diffusion model.

Research Group

Chetan Gadgil, Supercomputing Institute Research Scholar

Magdalena Stolarska, Research Associate

Fernando L. Reitich, Principal Investigator

High-Order Methods for Computational Electromagnetics and Acoustics

These researchers have recently developed a variety of high-order numerical techniques for the simulation of electromagnetic- and acoustic-wave scattering processes in the time and frequency domains. The most significant theoretical and implementational aspects of the methodologies were completed using limited computational resources. This work demonstrated the viability of the newly developed schemes for scattering simulations and it also proved that they offer the potential for substantial improvement in simulation capabilities over currently available methods. The new procedures are based on high order and efficient treatments of integral and differential formulations of the scattering problem. These treatments, as the group has demonstrated in a wide array of test cases, significantly reduce the number of degrees of freedom needed to attain a desired accuracy while simultaneously retaining a reduced operation count. Confirming these advantages for some practical, realistic geometric arrangements at frequencies of interest demands the use of supercomputing resources. The researchers are using the supercomputers to improve and expand their current codes to efficiently run simulations of practical interest.

Research Group
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Gerardo Ortigoza, Graduate Student Researcher

Fadil Santosa, Principal Investigator
Gennady Lyubeznik, Co-Principal Investigator

Parallel Buchberger Algorithm

The Buchberger algorithm for computing a Grobner basis of an ideal in a polynomial ring may be viewed as a generalization of Gaussian elimination for systems of linear equations. Research into this algorithm shows that the upper bound of both space and time complexity is double exponential in the number of variables, and this bound is reached in the worst cases. In the "generic" case, the amount of work to be done by the algorithm is believed to be unpredictable.

The nature of the Buchberger algorithm is sequential, thus allowing not much room for parallelization. However, over the years mathematicians and computer scientists have developed several approaches to parallelize it. All of them displayed certain speedups in computations, but, unfortunately, none of these theoretical methods has become practical.

These researchers are developing another parallel version for the Buchberger algorithm in a "slightly noncommutative" setting. That is, instead of the ring of polynomials, they deal with an associative algebra called Weyl algebra, in which not all of the variables commute. Partial results show that speedups superior to those of the commutative case are possible. The researchers are using supercomputing resources in order to test their code on as many processors as possible in order to understand the behavior of the parallel algorithm. Memory requirements are rather high also because of the so-called intermediate expression swell that occurs in the Buchberger algorithm.

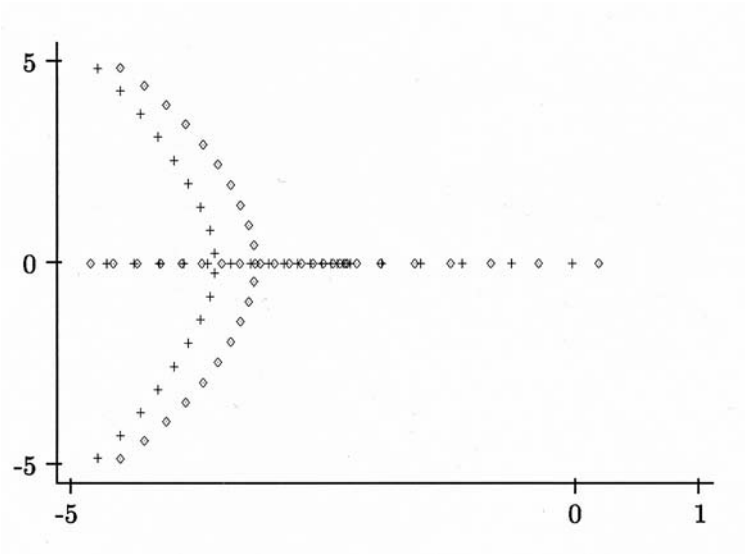
Research Group
Anton Leykin, Graduate Student Researcher

Arnd Scheel, Principal Investigator

Instability of Waves in Spatially Extended Nonlinear Reaction Diffusion Systems

Instabilities of excitation pulses have been observed in various experiments and related reaction-diffusion systems. Phenomenologically, secondary pulses grow out of the wake of a primary pulse. These may travel in the opposite direction as the primary pulse (backfiring) or in the same direction (trailing waves/tracefiring). Numerically, this has been observed in models of carbon oxidation on platinum, the Belousov-Zhabotinsky reaction, and models for physiological calcium flow. Experimentally related phenomena have also been found, in action potential dynamics of mutated nerves, for example.

These researchers are using supercomputing resources to corroborate an abstract bifurcation model, which requires extensive spectral computations on large domains near the instability threshold. Some preliminary results are shown in the figure. The structure of the critical spectrum of the pulse with separated boundary conditions behaves in good agreement with the researchers' theoretical predictions: near threshold, several eigenvalues are created by the increasing oscillations of the tail and move towards the unstable half plane. However, the spectral computations also show clusters of eigenvalues in the stable half plane, where theory predicts only finitely many, isolated eigenvalues. The researchers believe that this is caused by a bad behavior of the resolvent, which makes spectral computations of these very large matrices unreliable in certain regions of the spectral plane. In fact, theory predicts that in regions bounded by the essential spectrum, the resolvent behaves badly, although eigenvalue clustering only occurs at curves of absolute spectrum. Bad behavior of the resolvent is caused by symmetrizers with coefficients that are exponentially small in the size of the domain. The researchers will therefore use (physically unrealistic) periodic boundary conditions together with theoretical predictions for the essential spectrum to detect possible isolated eigenvalues.



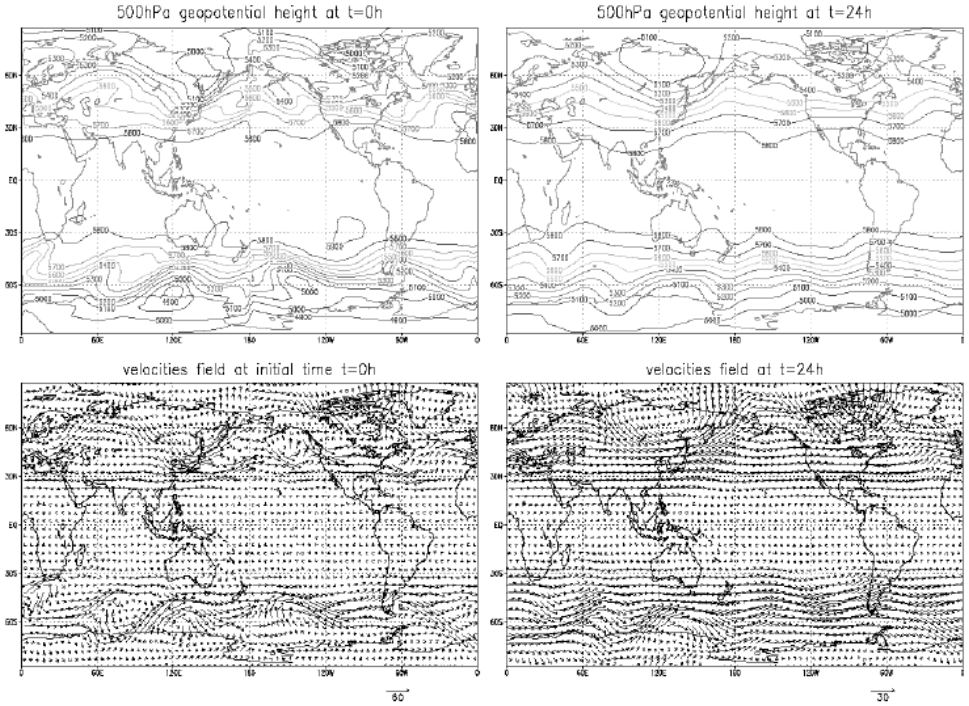
Critical spectra of the primary pulse in stable regime (crosses) and close to instability (diamonds).

Research Group

Jens Rademacher, Graduate Student Researcher

Douglas N. Arnold, Fellow

Optimal Integration of Atmospheric Chemical Transport Models and Measurements Through Variational Data Assimilation



The configuration of the model state, 500hPa geopotential height and velocities field, at the initial time t=0 hr and after a 24 hr forecast. A significant forecast improvement may be achieved by deploying adaptive observations in time varying regions where the model forecast is highly sensitive to parameter variations.

Chemical transport models (CTMs) are designed to describe physical and chemical processes in the atmosphere and their integrated impacts on atmospheric pollutant concentrations. The goal of this project is to develop computational tools and associated software for assimilation of atmospheric measurements into CTMs using the adjoint modeling and optimal control theory. Four-dimensional-variational data assimilation techniques are used to produce three-dimensional, time-varying, optimal representations of the chemical composition of the atmosphere that are consistent with the observed physical and chemical states.

Successful use of the four-dimensional-variational framework requires efficient solutions to computational problems including construction of the adjoint model, evaluation of the gradients by reverse integration, optimal storage and checkpointing schemes, and optimization. The resulting data assimilation problem is an intensive computational process that requires supercomputing facilities and makes parallel computing an ideal environment for air quality modeling.

Research Group

Dacian Daescu, Supercomputing Institute Research Scholar

Avram Bar-Cohen, Principal Investigator

Compact Modeling of Heat Sinks

The increasing complexity of electronic systems has resulted in increased computational effort in computational fluid dynamics (CFD) modeling. Computational effort and design time can be reduced by the substitution of the detailed heat sinks with "porous block" compact heat sinks in the CFD model. These researchers are developing a compact modeling methodology to determine the thermofluid properties of the compact heat sink to ensure desired accuracy in the temperature and pressure fields. Since a wide range of heat sinks can be used in a variety of conditions, this methodology has to be generic. Therefore, the researchers considered a wide variety of parametric dimensions such as heat sink type (parallel plate, pin fin arrays), separation between heat sinks, and flow regimes (laminar, turbulence).

Supercomputing resources were used to create a boundary layer methodology that successfully determined the compact heat sink porosity and the pressure drops of shrouded, parallel plate heat sinks in laminar forced convection. The researchers also derived an expression for thermal conductivity to obtain agreement in base temperatures of the compact and detailed heat sinks. This methodology has been extended to different parallel plate and pin fin heat sinks, different spacings between heat sinks, and different flow velocities in the laminar flow regime.

During this research period, the Bar-Cohen group extended the loss coefficient methodology to unshrouded heat sinks with flow bypass around the parallel plate heat sinks and the pin fin heat sinks. Some of the fast-moving flow bypasses the heat sink owing to its higher flow resistance. As a result, the pressure drop across the heat sinks will be lower than that of the fully ducted heat sink. For the same reason, the heat sink base temperatures are also higher compared to fully shrouded heat sinks.

With their success in compact modeling of fully shrouded and unshrouded compact heat sinks for plate and pin fin arrays, the researchers plan to test the universal applicability of compact modeling methodology in high speed turbulent flows.

Research Group

Karl J. Geisler, Graduate Student Researcher
Sridhar Narasimham, Graduate Student Researcher
Gary L. Solbrekken, Graduate Student Researcher

John C. Bischof, Principal Investigator

Numerical Simulation and Optimization of Thermal and Injury Behavior During Multi-Probe Cryosurgery of the Prostate

Cryosurgery has been used to treat prostate diseases since it was introduced in the 1960s. In order to treat a large volume of diseased tissue, as occurs in prostate cancer, multiple probes have been used widely in recent years.

These researchers have built and solved a three-dimensional numerical model that mimics the clinical situation of prostate cryosurgery. The model, which uses the software package ANSYS, is a very useful tool to predict thermal response during this surgical procedure. The model allows the user to optimize the probe positions and treatment time to ensure complete killing of the diseased tissue while maximally saving the normal tissue surrounding it. The model is also helpful for understanding the injury mechanism of cryosurgery.

These researchers have also begun to investigate the thermomechanical response during multiple-probe cryosurgeries. Several experimental observations have suggested that mechanical injury also exists under certain extreme thermal conditions. This mechanical injury is caused by micro- and macro-cracking due to thermal stress inside the frozen tissue. The researchers are building a structural model to predict thermomechanical behavior resulting from the thermal expansion or contraction of prostate tissue. The results from the thermal model will be used as the input for the new model.

Research Group

Xiaoming He, Graduate Student Researcher

Jane H. Davidson, Associate Fellow

Corona-Enhanced Chemical Vapor Deposition of Silicon Dioxide in Indoor Electrostatic Precipitators

Corona discharges in air are the source of ions and electrons necessary to many pollution-control and industrial processes, including control of airborne particles, treatment of flue gases, decomposition of volatile organic solvents, water treatment, and surface treatment of polymer films and fabric. The corona plasma is a non-equilibrium plasma in which high-energy electrons induce chemical reactions even at room temperatures. Some of these are desirable, but others are unwanted. For example, corona-enhanced chemical vapor deposition (CVD) of insulating material on the corona discharge electrode suppresses the corona. One example is deposition of silicon dioxide on the discharge wires of indoor electrostatic precipitators. The silicon source is semi-volatile silicone used in personal care products. Electron-impact collisions ionize and/or dissociate silicon source molecules. The reactive "precursors" formed in these homogeneous reactions then move to the corona discharge surface and undergo heterogeneous reactions that produce SiO_2.

The objective of this research is to model the corona plasma and the global gas phase reaction that is the rate-limiting step in the deposition process. The researchers have previously modeled the electron number density and kinetic energy distributions in the positive direct current (DC) corona plasma. During this research period, they modeled the electron distribution in the negative DC corona plasma and simulated the ozone production in the positive and negative corona plasmas using the program FLUENT.

A new project begun during this period involves the study of heat transfer of air flowing across shaped tube heat exchangers. Polymer heat exchangers are an attractive alternative to metal heat exchangers in several applications in the transportation industry. One drawback of these devices is their low thermal conductivity. This negative impact can be overcome if methods to enhance the convective heat transfer rates can be found. The traditional approaches used to enhance heat transfer in metal heat exchangers are not effective for polymeric materials.

The objective of this project is to model the convective heat transfer rates for gases in various heat exchanger geometries that the researchers hope will result in enhanced heat transfer rates. The focus is on heat exchangers made of many small-diameter tubes. The researchers are considering tubes of various shapes, including lenticular, ogive, oval, and teardrop. FLUENT is used to model the temperature and flow field in the gas flow around these tubes. The results for individual tubes indicate that, compared to a circular tube, the lenticular tube enhances heat transfer by up to 20% and reduces pressure drop by about 30%. The next step is to simulate forced convection heat transfer across heat exchangers made of many tubes. The researchers wish to find the effects of the arrangement of the tubes, tube pitch, and tube shapes on heat transfer and pressure drop. Other options under consideration include tube bundles made by interlacing the flexible tubes and weaving the tubes with fine threads to create local vorticity.

Research Group

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Meghan Kearney, Graduate Student Researcher
Mike Kingsley, Graduate Student Researcher
Zhihua Li, Graduate Student Researcher
Wei Lu, Graduate Student Researcher

Sean C. Garrick, Associate Fellow

Large-Scale Simulation of Turbulent Transport

Nanoparticles play an integral role in a wide variety of physical/chemical phenomena and processes. These include synthesis of nanostructured materials, including nanoparticles and coatings. The market for nanomaterials has dramatically increased in recent years with the growth of applications in industries such as microelectronics, cosmetics, chemical gas sensors, capacitors, and heat and mass transfer, among others. Nanostructured materials are expected to play an increasingly significant role in many major industries.

There are several technologies that can be employed in the manufacture of nanoscale materials (films, particles, etc.). However, the vapor-phase methodology is by far the most favored because of chemical purity and cost considerations. The formation of very fine particles from vapor encompasses a large number of physical and chemical phenomena. When driven from gas phase precursors (as is typical in many cases), over some time-temperature history, one must account for vapor phase chemistry, nucleation, and subsequent growth (coagulation/coalescence). The exact mechanisms are complex physico-chemical interactions that must include hydrodynamic mixing.

The goal of this project is to draw upon expertise in the fields of computational fluid dynamics, aerosol dynamics, chemistry, and physics to develop computational tools to simulate particle formation and growth in turbulent reacting flows. The methodology unites the latest mathematical and phenomenological models with robust simulation techniques, thus creating a new regime of computational flow physics/chemistry. This new approach will facilitate the prediction and control of nanoscale particle production for materials processing.

Research Group

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Nelson Settumba, Research Associate
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Steven L. Girshick, Associate Fellow

Modeling Plasma Synthesis of Materials

These researchers are performing numerical modeling of industrially important systems in which thin films or particles are synthesized from the gas phase. Key issues include the detailed chemistry that governs film growth, and the nucleation, growth, and transport of particles in plasmas. There are four main projects contained in this research.

One project investigates particle formation and transport in semiconductor processing systems. 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. These researchers are developing approaches for modeling particle formation, growth, charging, coagulation, and transport for these industrially relevant processes. The goal of this work is to develop and integrate particle nucleation and growth models with transport models of the processing environment. The researchers have developed detailed reaction mechanisms describing silicon clustering chemistry in the silane-hydrogen system and have coupled these to models of the reacting flow and particle growth and transport during the thermal chemical vapor deposition of silicon films. This model has recently been substantially extended to account for plasma chemistry, for conditions typical of low-pressure silane plasmas. The group has also begun to develop models of the deliberate deposition of amorphous hydrogenated silicon films with nanocrystalline inclusions. The inclusions come from particles that nucleate in the gas phase and then are transported to the film surface. The interest in these materials is for solar cell applications, as the presence of the inclusions has been shown to improve the material's stability against light-induced defect creation. These films are grown in silane-hydrogen plasmas, at pressures somewhat higher than those used for conventional plasma-enhanced chemical vapor deposition (CVD) of silicon.

Another project involves synthesis of nanostructured materials in a thermal plasma expansion process. Nanophase materials show reduced sintering temperature, increased hardness, and interesting electronic and optical properties. These researchers have 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 of the nozzle by inertial impaction. The researchers are developing this process in two modes: for the deposition of continuous films over large areas, and for the deposition of lines and patterns by using aerodynamic focusing to create nanoparticle beams.

The researchers are also performing fundamental studies of thermal plasma chemical vapor deposition. After concluding a project with diamond, they have begun studying thermal plasma CVD of hard ceramic materials, particularly silicon carbide and boron carbide. As part of this new project, the researchers have designed a completely new experimental reactor, and have developed models to predict the flow and temperature distributions in this reactor. They have performed a preliminary numerical modeling of flow and chemical compositions in the reactor for the Si-C-Cl-H system, and are beginning to develop detailed numerical models of the chemically reacting boundary layer at the growth surface for the chemical system B-C-Cl-H. This activity includes the generation, where necessary, of thermochemical property data and rate constants using *ab initio* quantum chemistry models.

Finally, in a new project, the researchers are studying the synthesis and energetic properties of nanoparticles of materials such as aluminum. They

Continued on next page

Steven L. Girshick, Associate Fellow

Research Group

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Bo Liu, Graduate Student Researcher
Soonam Park, Graduate Student Researcher
Song-Moon Suh, Graduate Student Researcher
Sarah Warthesen, Graduate Student Researcher

have developed an experimental system in which aluminum nanoparticles are synthesized in a direct current plasma expanded through a subsonic nozzle, which then encounters a cold counterflow that quenches coagulation. The particle surfaces are subsequently passivated by heterogeneous reactions, driven by ultraviolet (UV) radiation from UV lamps, in order to grow thin polymer or other passivating coatings. The researchers are developing computational models of this entire process, including the flow, particle nucleation and growth, and surface passivation.

Richard J. Goldstein, Associate Fellow

Heat Transfer at High Rayleigh Number

These researchers are analyzing natural convection and heat transfer in high-pressure conditions, which require a high Rayleigh number. Flow and heat transfer regimes at high Rayleigh number (~$O(10^{15})$) in a Bernard convection cell are numerically simulated using a spectral/Chebyshev collocation method. Rayleigh numbers at which transitions in the behavior of the Nusselt number occur are identified, and the mechanisms responsible for such transitions are studied. To convert the mass transfer coefficient to the heat transfer coefficient, an analogy factor between the heat transfer and mass transfer is needed. Usually, this is measured on a flat plate. For complex geometries, the analogy factor currently can be measured only by experiment. These researchers are planning to calculate the analogy factor and compare it with experimental results.

Research Group

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Joachim V. Heberlein, Associate Fellow
Emil Pfender, Co-Principal Investigator

Plasma Computation

Plasma processing is increasingly being used to develop new materials-processing technologies and to improve existing ones. Process models may be used as design tools to simulate complex phenomena, such as magneto-fluid-dynamic interactions, turbulence, and particle breakup and transport, that take place in processes such as wire-arc spraying, plasma deposition, and plasma spraying.

A computer code for the accurate calculation of thermodynamic and transport properties of different plasma mixtures has been developed and is being modified. These transport properties will be used to simulate the various processes mentioned above. All the projects involve the iterative or transient solution of a large set of strongly coupled non-linear equations, often with a very fine grid resolution in a two- or three-dimensional geometry, and thus require the resources of the Supercomputing Institute.

During this research period, the researchers:

- Updated the property program to obtain more reasonable properties of plasma mixtures.
- Computed plasma characteristics of a direct current (DC) high-intensity arc in two- and three-dimensional domains with a cross flow, and compared them with experimental data.
- Obtained new results revealing the significant three-dimensional effects inside a non-transferred DC arc plasma torch.
- Developed parallel codes for modeling of kinetic and chemical non-equilibrium in transferred DC arc plasmas.
- Analyzed the three-dimensional transient phenomena concerning heating of two ceramic cylinders by an electric arc with phase change.
- Analyzed voltage variations measured in a DC non-transferred plasma torch and developed a numerical model to describe the observed instabilities.

Research Group

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He-Ping Li, Research Associate
Joon Park, Graduate Student Researcher
Martin Vysohlid, Graduate Student Researcher

Uwe R. Kortshagen, Associate Fellow

Highly Realistic Modeling of Low-Pressure Processing Plasmas

This project is concerned with new approaches for fast realistic modeling of low-pressure processing plasmas. One focus of the project is the accurate prediction of the electronic energy distribution function, which is essential for the correct prediction of atomic processes and plasma-chemical rates in low pressure plasmas. Approaches relying on the numerical solution of the Boltzmann equation frequently have to use a number of approximations and are limited in their range of validity. This group uses a highly realistic Monte Carlo approach that is based on first principles to accurately determine the electron energy distribution function in a low-pressure plasma. The results of this research provide insight into the physics of electron transport processes both in configuration and in energy space. The benchmark calculations performed also serve as reference for comparisons with less general methods based on the approximate numerical solution of the Boltzmann equation.

The second focus is the study of the chemical nucleation of nanometer-sized particles in plasmas. This part of the project is focused on the chemical nucleation of clusters. The researchers are developing plasma-chemical reaction mechanisms that include neutral as well as ion-neutral chemistry. These efforts have yielded new insights into the chemical nucleation pathways in silane and acetylene plasmas. A recent result of this work relates to the experimentally observed fact that initial particle growth in low-temperature argon-silane plasmas is strongly affected by surrounding gas temperatures. This group's model predicts that this is due to temperature dependence of the Brownian diffusion coefficient. Both growth rates and loss rates of particles are affected by diffusion such that loss rates are increased and growth rates are slowed with an increase in temperature. This leads to an adverse effect on the overall particle growth rate, significantly slowing it.

Research Group

Upendra V. Bhandarkar, Graduate Student Researcher
Lorenzo Mangolini, Graduate Student Researcher
Peng Zhang, Graduate Student Researcher

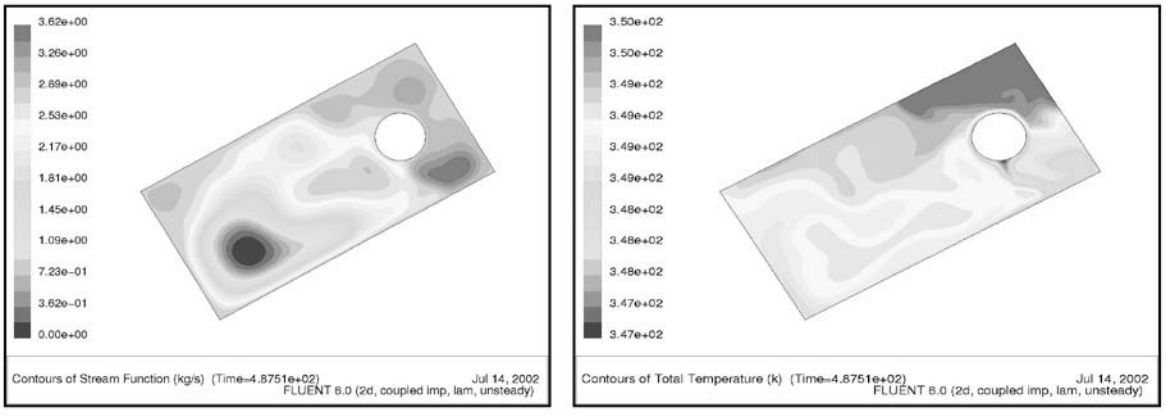
Francis A. Kulacki, Principal Investigator

Unsteady Free Convection and Stratification in Tilted Enclosures

These researchers are examining thermal storage devices, such as might be used in solar energy systems, from a generic viewpoint. A two-dimensional enclosure tilted at 30 degrees with a length-to-height aspect ratio of 2:1 discharges energy to the cold pipe located near the upper edge of the enclosure, while all the boundaries of the enclosure are perfectly insulated. This situation represents an integral collector storage system that is a proposed solar energy technology. The cold tube is the simplest heat exchanger that can be envisioned for withdrawing heat stored in the enclosure that receives energy from the sun at its upper surface. A numerical solution using a finite volume numerical procedure is employed to develop a fully parameterized solution for laminar flow when the boundaries of the enclosure have no thermal capacity and are not conjugated to the flow. Results are presented in terms of the enclosure Rayleigh number and a thermal modulus that scales the heat flux to the bulk temperature of the enclosure. Results to date include streamlines, velocity contours, and temperature fields for a system with a constant temperature tube and an enclosure fully charged to a uniform temperature. Local and average heat transfer rates to the tube as a function of time and angular position on the tube are being tabulated, and an overall heat transfer correlation is being sought in the equation $Nu_D = CRa^n$, where Nu_D is the Nusselt number based on tube diameter and Ra is the Rayleigh number. The researchers have found that the typical discharge time is 10–15 hours and Rayleigh numbers are $10^6 < Ra < 10^8$. Continuing work addresses an enclosure of aspect ratio 8:1 and the effect of a non-circular pipe, such as one with an octagonal cross section.

Research Group

Varaprasad S. Allumallu, Graduate Student Researcher



Streamline (left) and temperature (right) contours in a 2:1 initially isothermal enclosure during discharge at t=487.5 seconds after the start of the thermal transient. Streamlines are dimensionless and temperatures are in degrees Kelvin (K). The tube wall is isothermal, and the working fluid in the enclosure is water.

Perry Y. Li, Principal Investigator

Optimization of Flow Forces in Hydraulic Valves; Numerical Experimental Platform for an Aquatic Vehicle

This research group is involved in two major areas involving fluid flow. The first project studies fluid flow in electrohydraulic valves to determine a design that maximizes the valves' performance. The goal of the second project is to design novel propulsion systems for aquatic vehicles.

Hydraulic systems are heavily used in agricultural, construction, manufacturing, material and structural testing, and entertainment industries. The control of hydraulic systems involves the operation of an electrohydraulic valve in which a spool is stroked within the valve sleeve using a solenoid stroking actuator, in order to mechanically meter the fluid flow into and out of the hydraulic piston. A determinant of the dynamic performance of such systems is the speed and rate at which the spool can be stroked. For high flowrate, high bandwidth applications, the flow forces that the solenoid needs to overcome in order to move the spool become significant, thus limiting the performance of the valves. This project aims to overcome this difficulty by designing the geometry of the spool so that, as the fluid flows through the valve, the fluid flow induced forces on the spools are open-loop unstable. Potentially, a very small solenoid stroking actuator can be used in conjunction with a controllable brake to achieve very high speed operation of the electrohydraulic valves.

The researchers are using the computational fluid dynamics (CFD) program FLUENT to help them understand the flow field inside a hydraulic valve and how the valve geometry affects the transient and steady flow forces. They have evaluated and validated both the steady state and transient flow forces that arise inside the valves. These results are consistent with the researchers' hypothesis that, by varying the damping length of the valve, the transient force can be made to be unstable, thus enhancing the agility of the spool. The analysis also confirms that fluid viscosity can also be used to improve the agility of the spool, by countering the stable effect of the steady flow forces. The researchers are now using multiple CFD analyses to determine definitive simplified valve design models.

The second project takes its inspiration from the method aquatic animals use to swim to design novel propulsion systems. Specifically, the project's goal is to achieve highly efficient, highly maneuverable propulsion for aquatic vehicles using an oscillating foil as a propulsor. A key factor in this study is to understand how vortex generation, propagation, and roll-up affect the dynamics of the aquatic vehicle. The researchers are using the supercomputers to run a numerical simulation platform that simulates the fluid flow, vortex interactions, and the dynamics of the aquatic vehicles. "Blob" (Rossi) codes in which vortex combinations are performed for efficient time stepping have been extended for this project.

Research Group

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Kumaragovindhan Santhanakrishnan, Graduate Student Researcher
Qinghui Yuan, Graduate Student Researcher

Peter H. McMurry, Associate Fellow

Modeling of Particle Transport in High-Density Plasma Chemical Vapor Deposition Tools

The goal of this project is to create models to help avoid particle contamination in the manufacture of semiconductors. 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 2005 particles down to 0.050 μm, and perhaps as small as 0.015 μm, will be critical to the yield of 1 Gbit Dynamic Random Access Memory computer chips. Such ultrafine particles are typically produced by nucleation in the gas phase. The main objective is to develop computational models to predict particle transport generated by nucleation in high-density chemical vapor deposition tools.

During plasma processes, particles are charged negatively due to higher electron flux and trapped inside the plasma electrostatically. The purpose of this project is to predict the particle trajectory after the plasma is turned off. The flow velocity and temperature field were obtained first by using FLUENT. Then, the particle trajectories were calculated by simulating a discrete second phase in a Lagrangian frame of reference.

The results of this modeling work will be compared to those of experimental work that uses transmission electron microscopy. The combined results will improve the understanding of particulate contamination during semiconductor fabrication and will eventually make it possible to develop novel strategies to achieve defect-free manufacturing of semiconductor devices.

Suhas V. Patankar, Fellow

Microscopic and Macroscopic Simulations of Flow and Heat Transfer in Periodic Porous Media

This project includes developing and applying computational techniques for fluid flow, heat and mass transfer, turbulence, radiation, chemical reaction, and related purposes. The researchers incorporate flexible and efficient numerical techniques into general-purpose computer programs, which are used for the numerical simulation of practical problems. Recent and ongoing investigations have focused on heat transfer on gas turbine blades, oscillating turbulent flow in pipes, natural convection in enclosures, various techniques for heat transfer enhancement in heat exchanger passages, film cooling of combustion chamber walls, vortex shedding behind cylinders, buoyant plumes, and flow in porous media. The computational work is carried out in order to understand complex physical processes. The computed results, therefore, not only provide useful quantitative information for design, but also lead to better insight into the heat transfer and fluid flow mechanisms. Supercomputing Institute resources are necessary for these calculations because of their complexity and demanding computational load.

These researchers have constructed a database of flow resistances for a range of Reynolds numbers and flow directions by computation of the microscopic model. The resistances database is used in the calculations of the macroscopic model. The macroscopic model solutions have been compared to direct simulations in terms of velocity profiles, stream functions, and pressure drop. Preliminary hydrodynamic characteristics results obtained from the microscopic and macroscopic simulations of flow in modeled porous media are found to be in excellent agreement with the results obtained from direct simulations. These results demonstrate the efficiency and robustness of the two-model approach in simulating periodic porous media.

Research Group

Aiman Alshare, Graduate Student Researcher
Kanchan Kelkar, Research Associate
Amir Radmehr, Research Associate

David Y. H. Pui, Associate Fellow

Dynamic Filtration Simulation of Pleated Filter Cartridges Under Pulse-Jet Cleaning in a Baghouse

Filter bags have been widely adopted in industry for pollution control for three decades. Many studies have been performed on the cleaning performance of flat filter sheets. However, pleated filter cartridges have recently attracted more attention, because their larger surface area means they have the potential for reducing the operating cost of the baghouse. Flat-sheet and pleated filter media have different filtration and cleaning characteristics, but relatively few studies in the literature have reported data relating to pleated baghouse filter operation.

These researchers are collecting experimental data on pleated filter cartridges, but they also will use numerical simulation to analyze the dynamic filtration process of a baghouse system including backpulse cleaning for the pleated filters. They are developing a model to help engineers understand and design the baghouse system. Supercomputing resources are necessary for this work because of the need to include parameters such as filter deformation during pulse-jet cleaning and the solution stability of air flow passing through the complicated pleat geometry of the filters.

Research Group

Liming Lo, Graduate Student Researcher
Se-Jin Yook, Graduate Student Researcher

Terrence W. Simon, Associate Fellow

Simulations of Flow and Heat Transfer in Complex Engineered Systems

These researchers continued their investigations into the numerical simulation of three complex-engineered systems: boundary-layer controls in external and mixed-compression inlets of supersonic aircraft engines; internal and film cooling of gas turbine components; and flow control in spark-ignited-direct-injection engines. Two types of simulations were performed. One type is based on the Reynolds-averaged Navier-Stokes (RANS) equations closed by low-Reynolds number turbulence models. The other type is based on large-eddy simulations (LES) in which only the sub-grid scales are modeled.

The long-term objective of this research has three parts. The first was to assess the effects of grid resolution and grid-quality measures by com-

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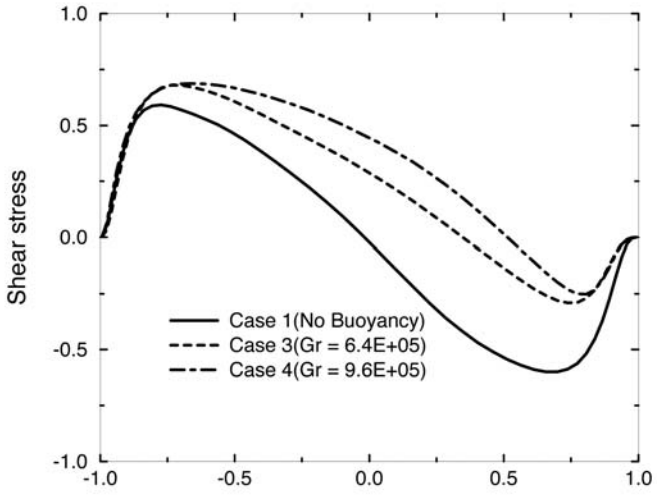

Distribution of resolved turbulent shear stress across a vertical channel heated on right side showing the effects of buoyancy on the stress.

Terrence W. Simon, Associate Fellow

Research Group and Collaborators

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paring predictions with grid-independent solutions. The second sought to evaluate the accuracy of RANS and sub-grid turbulence models by comparing predicted results with experimentally measured ones. Spatially resolved experimental data on mean variables in inlets are available from National Aeronautics and Space Administration (NASA)-Glenn and Boeing; spatially-resolved mean and variance data on gas turbine heat transfer are available from the researchers' laboratory at the University of Minnesota; and time- and spatially-resolved data inside internal combustion (IC) engine cylinders are available from Michigan State University. The third focus of this three-pronged objective was to extract understanding about the physical processes with the aim of using them to impact design.

During this period, these researchers obtained large eddy simulations of rotating channel and duct flow with and without heat transfer, using the sub-grid scale model. These results are important for applications such as cooling schemes for turbine blades in high performance jet engines. Rotation significantly alters the structure of turbulence in ways that are not well understood. The group also completed studies on the effects of buoyancy on flow and heat transfer in vertical pipe and annular passages.

Patrick J. Starr, Principal Investigator

One-dimensional and Two-dimensional Modeling of Dynamic Fluid Flow in a Four-Stroke Multi-cylinder Spark-injection Engine

This research project consists of using industry-standard one-dimensional and three-dimensional modeling software to improve engine performance by increasing volumetric efficiency. The project uses the Ricardo WAVE (one-dimensional) and VECTIS (three-dimensional computational fluid dynamics) software packages to model the dynamic flows within a four-stroke spark ignition engine.

The research focuses on compressible fluid flows through the intake and exhaust manifolds. Areas of investigation include cylinder-to-cylinder air distribution, taper/curvature of intake manifold runners, and pulsed choked flow through an orifice/venturi restrictor. The results of computer simulations will be compared with dynamometer experiments.

Adverse cylinder-to-cylinder intake air distribution limits the final output, efficiency, fuel economy, and emissions of any engine, and is a key factor in cycle-to-cycle variability. Engine designers go to great lengths to reduce this variability and to better understand the variables that create it. Similar computational methods are now being used by other researchers in industry and academia to explore exhaust gas recirculation distribution in a quest to lower emissions. The ultimate goal of this project is to use the WAVE and VECTIS software to increase understanding of adverse cylinder-to-cylinder air distribution, intake runner geometry, and pulsed fluid flow with the intent of improving real-world designs.

Research Group

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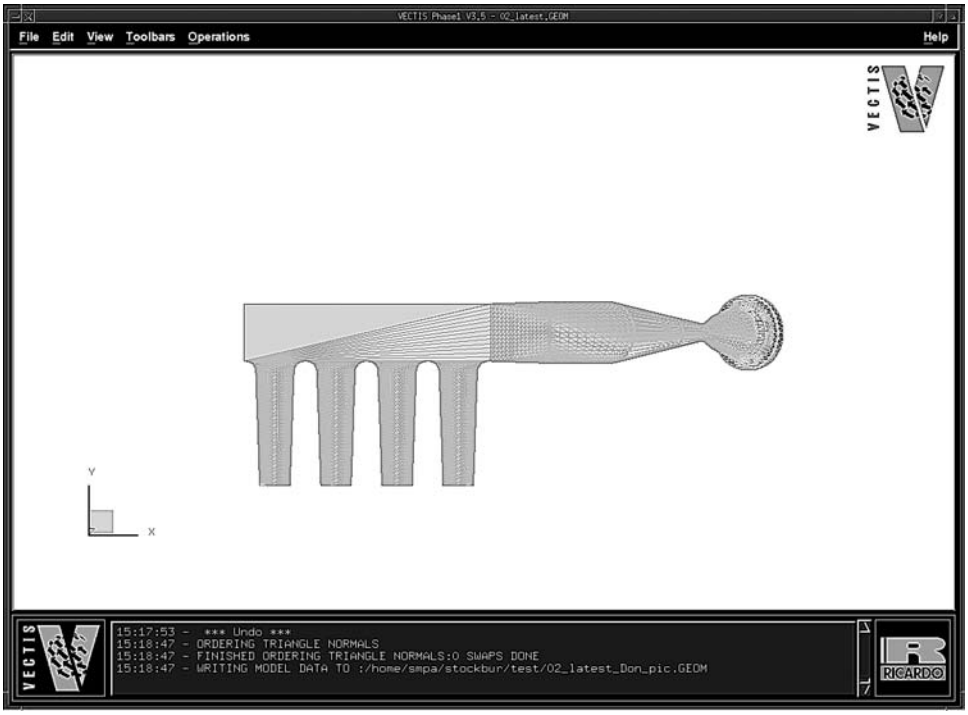
Garrett R. Stockburger, Graduate Student Researcher



This screen shot illustrates one of three research geometries used in the Vectis–Phase 1 program prior to "boundary painting" and meshing.

Kumar K. Tamma, Fellow

Applications of Supercomputing to Interdisciplinary Computational Mechanics

This research constitutes an effort toward the development of unified computational methodologies, solution algorithms, and finite element modeling/analysis strategies for multi-disciplinary flow-thermal-structural problems. The philosophy and rationale of this work 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. The application areas include a wide range of engineering problems involving multi-physics and space/time domain decomposition with interface to graph partitioning techniques.

These researchers are involved in the following specific projects:

- Materials modeling and manufacturing simulations to include structural performance by employing micro-macro integration for the multi-disciplinary interactions.
- Development of new time integration methodologies and approaches for structural and thermal analysis. These are based on unified Generalized Integration Operators (GInOs) employing robust time integration schemes based on discrete numerical markers.
- Analysis and modeling of fluid and thermal interactions existing in the solidification processes including the phase change effects that exist in processes such as precision molding and metal casting.
- Development of a contact model to include frictional effects. Impact and penetration analysis involving large-scale structures and large finite element models require a very large memory and computational resources.
- Application of a frictional contact model for manufacturing simulations involving metal forming processes and finite element methodology. The nonlinearities (both geometric and material) necessitate a need for large computing and memory resources and are critical.
- Analysis and modeling of flow, thermal, and reaction kinetics phenomena that exist during the manufacturing of composite materials in a concurrent engineering environment. The analysis involves macro and micro flows in a network of fibers and analytical prediction of permeabilities by appropriate flow models and fiber networks. Applications are targeted toward new massively parallel computing systems such as the IBM SP.
- Development of new finite-element-based methodologies that can be used in interdisciplinary problems.
- Investigation of thermal transient analysis involving moving boundaries, removal of

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Sha Desong, Graduate Student Researcher
Ramdev Kanapady, Graduate Student Researcher
Ram V. Mohan, U. S. Army Research Laboratory, Aberdeen, Maryland
Nam Ngo, Graduate Student Researcher
Sukpreet Singh Sandhu, Research Associate
Dale Shires, U. S. Army Research Laboratory, Aberdeen, Maryland
Anak Somkanae, Graduate Student Researcher
Ho Nguyen Tran, Graduate Student Researcher
Radu Valasutean, Graduate Student Researcher
Xiangmin Zhou, Research Associate

Kumar K. Tamma, Fellow

materials during processes such as ablation, and phase change issues in biological systems. These also involve re-meshing and adaptive meshing during the analysis, which require large amounts of computing time and memory.

- Multi-body dynamics and integration of stiff ordinary differential equations with constraints.

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.

Michael R. Zachariah, Principal Investigator

High-Temperature Chemistry and Physics of Vapor Phase Nanoparticle Growth and Microcombustion Processes

This research is aimed at using molecular-based computation to understand the growth of nanoparticles formed from the vapor and the high-temperature oxidation of hydrocarbons in microcombustors.

In one project, the researchers are performing classical molecular dynamics (MD) simulations to understand particle-particle interactions and properties. Specifically, these studies attempt to determine particle-particle reactivity and physical/chemical properties of small particles (surface tension, internal pressure, etc.) that are important in the growth of nanostructured materials. The research currently focuses on the simulation of silica particles using a two-body empirical potential. The researchers have developed a code that computes the pressure profile through a particle for particles up to 1,152 atoms. The current plan is to develop methods for the direct computation of surface tension from the pressure profile and observe the particle size dependence of surface tension. The results from the MD computations are used to feed aerosol dynamics programs for tracking the ensemble growth of nanoparticles.

A new project involves building a MicroElectrical Mechanical Systems (MEMS)-based combustion engine as a high density portable electric power source. As part of this work, the researchers are developing models that can simulate the fluid flow and combustion chemistry in a MEMS combustor. These simulations involve solution of coupled flow, heat/mass transfer, and detailed chemistry. These models will be a great help in the design of the prototype combustor, but perhaps more importantly will help the researchers explore a wide variety of fundamental problems related to reacting flow in microreactors. In addition, the researchers are developing a model for a free piston engine that will incorporate detailed chemistry with a time varying reactor volume that will allow them to model a piston movement and its influence on the chemistry and vice versa.

Research Group

Hans Aichlmayr, Graduate Student Researcher
Soo Hjung Kim, Graduate Student Researcher
Dibyendu Mukherjee, Graduate Student Researcher
Takumi Hawa, Research Associate
Irina Schwiegert, Research Associate
Shekar Sonwane, Research Associate

Charles E. Campbell, Associate Fellow

Micromagnetic Simulations

These researchers are continuing their work with micromagnetic simulations, which are simulations of magnetic material on the length scales of between several nanometers and several microns. The objective of these simulations is an understanding of the dynamics, the domain structure, and the structure of domain walls of useful magnetic materials such as permalloy, Ni, Fe, Co, and FeCo.

One project concerns the dynamics of permalloy thin films. The research group of E. Dan Dahlberg has created a five-micron square permalloy thin film, which has been examined by the group of Paul Crowell using the magneto-optical Kerr effect (MOKE) to obtain the magnetodynamics of this system. This is the smallest sample that they have been able to make or expect to be able to make with current technology, although there are some improvements in its squareness and reduction in thickness that may be possible. The first MOKE experiments show very encouraging similarities to the micromagnetic simulations of one- and two-micron square permalloy films. The researchers plan to extend their work to simulate the five-micron systems, thus permitting simulations and experiments to be run on very similar systems.

Also in conjunction with the Dahlberg group, these researchers are exploring the possibility of using small arrays of magnetic nanoparticles for digital electronics. One possible method is to apply this approach to nanoscale arrays of single crystal magnetite to simulate then experiment on logic elements driven by magnetics.

In addition to this work on magnetism, these researchers have begun a new project to simulate a multi-component diffusion conversion, the fox and rabbit problem, using cellular automata.

Research Group and Collaborators

Jesse Berezovsky, Undergraduate Student Researcher
Paul Crowell, Faculty Collaborator
E. Dan Dahlberg, Faculty Collaborator
Dave Engebretson, Graduate Student Researcher
Andrew B. Kunz, National Institute of Standards and Technology, Gaithersburg, Maryland
Ming Yan, Graduate Student Researcher

Eric D. Ganz, Principal Investigator

Molecular Modeling of Tripycene-Related Molecules on Si(001) Surfaces

These researchers are studying the geometric, electronic, and mechanical properties of molecular gear compounds, such as triptycene analogs, on silicon surfaces using the GAUSSIAN software package. The simulations will be compared to ultra-high vacuum scanning tunneling microscopy imaging of these molecules on the silicon surface. The simulations will also be used to design new gear molecules for these experiments. The large size of the molecules coupled to an Si cluster (to emulate the silicon surface) requires the use of supercomputing resources to ensure reliable results.

Research Group
Shimin Hou, Research Associate

Alexander Y. Grosberg, Fellow

Computer Simulations of Cooperative Behavior of Biopolymers

These researchers are working on projects concerning molecular dynamics simulations of charge inversion and the properties of compact polymer chains.

Charge inversion is the recently discovered counterintuitive phenomenon in which a charged macroion, such as a polymer or a colloidal particle, absorbs so many counterions that it effectively "flips" its charge sign. Charge inversion is important in a number of naturally occurring phenomena, such as nucleosome self-organization. It also has a vast array of practical applications, ranging from deoxyribonucleic acid (DNA) electrophoresis to gene therapy. Experimental studies of charge inversion are associated with significant difficulties, so molecular dynamics (MD) simulations have become the method of choice.

These researchers have made significant progress in their MD simulations of charge inversion, and are extending their simulations to include more realistic models, such as several of the macroions in the simulation domain. They are also increasing the volume fraction of surrounding solvent molecules so that it is closer to realistic values. This has importance for the practical questions arising in the field of gene delivery.

Another project involves investigation into the properties of compact polymer chains. The researchers developed an algorithm for random generation of the large compact self-avoiding walks on the cubic lattice. The researchers are applying this algorithm to the study of the entropy of the knots in the globular polymer rings and the correlation of the chain ends in the compact conformations of the linear polymers. They are studying how these properties of the polymer globules scale with the length of the chain.

Research Group and Collaborator
Alexander Borovinskiy, Research Associate
Rhonald Lua, Graduate Student Researcher
Nathan Moore, Graduate Student Researcher
Motohiko Tanaka, National Institute for Fusion Science, Toki, Japan

J. Woods Halley, Fellow

Numerical Studies of Fluids and Disordered Solids

This group is involved in three principal projects:

- Simulation of the electrode-electrolyte interface, including the dynamics of the molecules during electronic transfer to or from the electrode, and the study of the electronic structure of oxides and metals at the electrode-electrolyte interface using self-consistent tight binding molecular dynamics as well as *ab initio* plane wave techniques.
- Study of solvation, transport, and ion pairing in polymer electrolytes by molecular dynamics techniques.
- Calculations of properties of superfluid helium four and dilute Bose-Einstein condensed systems.

These studies have technical applications to corrosion, solar cell development, batteries, fuel cells, and nuclear waste disposal.

The simulation of electrochemical interfaces is one of a larger class of materials-related simulation challenges in which one needs to couple calculations spanning about 10 orders of magnitude in length and time scale in order to produce macroscopic predictions. Generally, methods within each scale are available, but robust and reliable methods for coupling one scale to another are not. In the group's work, methods for coupling the electronic structure scale to the atomic scale and the atomic scale to higher length scales were developed. At the electronic scale, both quantum chemical, Hartree-Fock-based methods, and solid-state, density functional methods—while working from the same principles—are used. Results from these electronic scale calculations are then used to parameterize models at the atomic scale, either as force fields for classical molecular dynamics calculations or as self-consistent tight binding models. Using these methods, the group has studied such features of electrochemical interfaces as electron transfer rates, capacitance, and oxide structure and conductivity. Intermediate-scale tight binding methods also made possible new kinds of study of magnetic solids and highly disordered solids, occurring in electrodes but also elsewhere. In the electrochemical studies, it is often also necessary to connect the atomic scale calculations to continuum models in order to make predictions of the experimental quantities of interest.

The study of polymer electrolytes is motivated by a worldwide search for better ion-conducting polymers for use in advanced batteries. The group previously has focused on molecular dynamics and Monte Carlo calculations of Li^+ and various anions in glassy polymers in order to study transport and ion pairing. They have now initiated related studies of proton transport. Using their model for amorphous polyethylene oxide, they developed a method for including the scattering of neutrons by hydrogen nuclei in the model to permit a direct comparison with the experiments. This comparison showed that the model's results corresponded well with experimental results. The group is studying the lithium ion's behavior and is putting together a global picture of the universal features of the mechanism by which lithium moves in this polymer.

The work on Bose-Einstein condensates was motivated by a search for better experimental probes of the condensate, particularly in liquid helium four. The group has investigated the helium vapor pulses used in their experiments. The simulations of high-power anomalous multiple-peaked signals use a hydrodynamic code with boundary conditions dynamically determined using a gas dynamics code, which has been recently developed to realistically model interatomic

J. Woods Halley, Fellow

scattering processes. This hybrid molecular dynamics/hydrodynamics code has not only achieved much faster running times, but has also shown the formation of shock waves that appear to give rise to the observed multiple peaks in the experiments due to interactions of the pulse with the ambient gas within the experimental cell. The hybrid code also offers the versatility of easily changing parameters, such as possible density profiles, to better match the conditions of the pulse experiments, and to predict how pulses might be generated to benefit the search for condensate mediation in a helium transmission experiment. The group has also begun an analysis of recent experiments they conducted in which they may have observed transmitted helium pulses through the superfluid.

Research Group and Collaborators

Nathan Baisch, Undergraduate Student Researcher
Jan Bording, Brookhaven National Laboratory
R. Chaudhury, Bose Institute of Science, Calcutta, India
Bach Thanh Cong, Solid State Physics Department, Hanoi University of Science, Hanoi, Vietnam
Yuhua Duan, Research Associate
Serkan Erdin, Supercomputing Institute Research Scholar
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Keith Lidke, Max Planck Institute, Gottingen, Germany
You Lin, Graduate Student Researcher
Rhonald Lua, Graduate Student Researcher
Dat Nguyen, Graduate Student Researcher
James R. Rustad, Battelle Pacific Northwest Laboratory, Richland, Washington
Patrick Schelling, Argonne National Laboratory, Argonne, Illinois
Herbert Shore, Department of Physics, San Diego State University, San Diego, California
B. Smith, National Renewable Energy Laboratory, Golden, Colorado
Mark Williams, Department of Physics, Northeastern University, Boston, Massachusetts
Aaron Wynveen, Physics Department, University of Wisconsin, River Falls, Wisconsin
Peter Zapol, Chemistry Division, Argonne National Laboratory, Argonne, Illinois
Weilin Zhang, Graduate Student Researcher
Min Zhuang, University of Montreal, Montreal, Quebec, Canada

Shaul Hanany, Associate Fellow

Data Analysis of Cosmic Microwave Background Experiments

These researchers continued their project to design and test the data analysis pipeline that will be used to analyze the MAXIPOL data set. MAXIPOL is a balloon-borne cryogenic experiment that is attempting to detect polarization in the cosmic microwave background (CMB). They have also compared temperature anisotrophy maps from the MAXIMA-1, MAXIMA-2, and ARCHEOPS experiments.

Research Group and Collaborators

Matthew Abroe, Graduate Student Researcher
Julian Borrill, National Energy Research Scientific Computing Center, Lawrence Berkley National Laboratory, Berkeley, California
Jean Christophe Hamilton, Physique Corpusculair et Cosmologie, College de France, Paris, France
Brad Johnson, Graduate Student Researcher

In preparation for the analysis of MAXIPOL data, the researchers have developed simulation software that computes a random realization of a cosmological model, and generates a CMB observation based on experimental parameters. They simulate a CMB observation by measuring the temperature and polarization on the maps according to the expected MAXIPOL observation strategy. This signal is then covolved with some finite beam pattern and random noise is added. The beam patterns and noise properties of the MAXIPOL detectors have been determined to high accuracy. This generates a vector of time stream data. From this vector, the researchers can compute the maximum likelihood temperature and polarization maps and power spectra, and compare those results with the initial cosmological model. The researchers have used these simulated data sets to test the polarization map-making code that will be used to analyze the MAXIPOL data set.

Norton M. Hintz, Principal Investigator

Nuclear Reaction and Structure Calculations

During the late 1980s and early 90s, this researcher performed experiments on proton elastic and inelastic scattering and two-neutron pickup reactions at the Los Alamos Meson Physics Facility and the Indiana University Cyclotron. The purpose was to investigate the basic nucleon-nucleon (NN) interaction as modified in the nuclear medium. There are several controversial and somewhat conflicting theories as to how the free NN interaction is modified by the presence of other nucleons. Fundamentally, the underlying quark structure of the nucleons is involved.

This purpose of this project is to analyze these data; these results have important applications in astrophysics, particle physics, and condensed matter physics. The analysis of the two-neutron transfer experiments has been completed and published, and the analysis of the proton inelastic scattering data is ongoing. The results of this work have important applications in astrophysics, particle physics, and condensed matter physics.

Robert L. Lysak, Associate Fellow

Numerical Investigation of Solar Wind-Magnetosphere-Ionosphere Coupling

The work performed by these researchers was centered on several problems involving the coupling of mass, momentum, and energy between the solar wind, magnetosphere, and ionosphere. This work involved both the development of new codes and the modification and use of existing codes to address the problem of solar wind-magnetosphere-ionosphere coupling. The emphasis was on magnetosphere-ionosphere coupling during magnetospheric substorms. The following is a summary of specific projects.

The researchers extended their model for describing the dynamics of the turbulent convective flow in the magnetospheric boundary layer using the three-dimensional version of the Total Variance Diminishing (TVD) magneto-hydrodynamic (MHD) code provided by the group of Thomas W. Jones of the Department of Astronomy. The main focuses during this period were an investigation of the nonlinear dynamics of the magnetospheric tail using this code, and the study of linear and nonlinear wave mode conversion at the plasma sheet boundary. In the first area, preliminary runs have studied the propagation of shear Alfvén mode pulses, which propagate along magnetic field lines. In these runs, two shear mode pulses propagating in opposite directions interact with each other. The interaction between these pulses depends on whether they have the same angular momentum and opposite helicity, or opposite angular momentum and the same helicity. Preliminary simulations support the expectations from theory that interactions with the same magnetic helicity create filaments in the field-aligned currents, while those with the same angular momentum create vorticity filaments that will be associated with charge holes. Furthermore, in both cases, plasma density depletions form during the interaction, although the depletions are stronger in the same helicity case. Such depletions are significant in the current-carrying plasma of the auroral zone, since parallel electric fields are enhanced in low-density regions. Although these simulations are still preliminary, they indicate that the dynamics of wave packets along field lines may play a significant role in auroral processes.

Research Group and Collaborators

James P. Crumley, Graduate Student Researcher
Thomas W. Jones, Faculty Collaborator
Kristi Keller, Laboratory for Extraterrestrial Physics, Goddard Space Flight Center, Greenbelt, Maryland
Dong-Hun Lee, Department of Astronomy and Space Science, Kyung Hee University, Korea
Yan Song, Research Associate
Akimasa Yoshikawa, Department of Earth and Planetary Sciences, Kyushu University, Fukuoka, Japan

The second application of the MHD/TDV code is the interaction of compressional waves with the plasma sheet boundary layer (PSBL), which is the interface between the dense plasma sheet and the magnetically-dominated tail lobes, which are very low-density plasma regions. Strong gradients in the Alfvén speed appear at this boundary, and theory predicts that mode conversion between the shear and fast modes should appear at this interface. Preliminary simulations have supported this prediction. The group also investigated the effect of magnetic shear at the PSBL interface to determine its role in breaking the symmetry in the wave conversion process.

Additionally, the researchers applied their three-dimensional model for the propagation of compressional and shear Alfvén waves through the auroral ionosphere and atmosphere by looking at the excitation and propagation of waves propagating in the so-called ionospheric waveguide, and by looking at the detailed structure of the ionosphere including collisional effects. A focus of this research was to incorporate the tilt of the magnetic field with respect to the vertical direction. The

Continued on next page

Robert L. Lysak, Associate Fellow

group has made the first steps in modifying the nonlinear MHD code described above to model the low-β plasma in the auroral acceleration region. They have also included the effects of ionospheric feedback.

Another aspect of their research concerned modeling wave propagation in the inner magnetosphere and coupling these processes to those in the geomagnetic tail and at the magnetopause. They are developing a model using non-orthogonal dipole coordinates to include the distortion of the geomagnetic field. This effort helps to describe the timing of magnetospheric phenomena during substorms as well as the propagation of the so-called Pi2 pulsations associated with substorms.

Lastly, the researchers performed particle-in-cell numerical simulations to describe the nonlinear evolution of so-called ion and electron holes that have been recently observed by the National Aeronautic and Space Administration Fast Auroral Snapshot (FAST) satellite. These phase space structures had previously been described theoretically in the steady state, but the evolution of such structures remains an open question. By implementing an Adaptive Mesh Refinement technique, the researchers hope to more efficiently simulate these structures. The recent focus of this work has been on searching for linear wave modes before the formation of the solitary waves in the simulations. In particular, the group wants to see if ion acoustic waves forming before the solitary waves are responsible for the formation of solitary waves, as proposed by some theories. So far, linear wave modes have not been observed, though turbulent fluctuations have been observed that support another theory that proposes the solitary waves forming from noise.

Oriol T. Valls, Fellow

Numerical Studies in Condense Matter Theory

These researchers are continuing their work in two main areas: proximity effects in superconductor/ferromagnet interfaces and structures, and study of the superconducting vortex system in the presence of pinning centers.

In the first area, recent developments in nanofabrication techniques have allowed researchers to create high-quality junctions between ferromagnets and superconductors. This has made it imperative to develop a theory of the proximity effects in these materials. There are two characteristic lengths: one involves the penetration of the ferromagnetism into the superconductor, and the other, conversely, the influence of the superconductor into the ferromagnet. The researchers have previously developed a method to numerically and self-consistently solve the exact relevant Bogolioubov-deGennes (BdG) microscopic equations in the continuum case. They are now using this method, at finite temperatures, to find the solutions of the BdG equations for experimentally relevant structures involving combinations of superconductors and ferromagnetic layers. The computational results will also be compared with experimental results.

In the second area, the researchers are continuing their study of the phase diagram of a superconducting vortex system with pinning centers. During this research period, they obtained results for the case of a regular pinning array, including the phase diagram and density distributions. The next emphasis is on the phase diagram of a system

Oriol T. Valls, Fellow

in the presence of random pinning centers, representing highly anisotrophic high temperature superconducting systems in an applied magnetic field. The researchers' method makes use of the free energy functional minimization numerical techniques that they originally developed to study hard sphere glassy systems. The inclusion of pinning centers is achieved through the introduction of a potential in the free energy used in the simulation. The free energy functionals include long-range interactions, in particular those derived from the Lawrence-Doniach free energy for layered superconductors.

Collaborators

Chandan Dasgupta, Faculty Collaborator
Klaus Halterman, China Lake Research Center, China Lake, California
Steve W. Pierson, Department of Physics, Worcester Polytechnic Institute, Worcester, Massachusetts
Igor Zutic, Department of Physics, University of Maryland, College Park, Maryland

Philippe de Forcrand, Adjunct Fellow

Quantum Chromodynamics at Finite Density

One prediction of quantum chromodynamics (QCD) is that quarks are confined at low temperature, but that a quark-gluon plasma forms above some temperature T_c. Current experiments on heavy-ion collisions may provide evidence for this plasma, and it is important to predict its properties. The critical temperature $T_c(\mu)$ depends on the relative excess of matter over antimatter in the heavy-ion collision, or equivalently on the quark chemical potential μ. Unfortunately, lattice QCD simulations can only directly probe the case $\mu = 0$, because otherwise the notorious "sign problem" prevents Monte Carlo sampling over a positive measure. These researchers have pursued an approach that is free of the sign problem, and that gives the most accurate results to date. In this approach, they use an *imaginary* chemical potential μ_I, for which standard Monte Carlo methods apply, and determine the critical temperature $T_c(\mu_I)$, then analytically continue its truncated Taylor expansion to real μ. The researchers are now using Supercomputing Institute resources to refine their results by pushing the Taylor truncation further and considering more realistic quark masses.

Collaborator

Owe Philipsen, Center for Theoretical Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts

Stephen S. Hecht, Principal Investigator

Biochemistry, Biology, and Carcinogenity of Tobacco-Specific *N*-Nitrosamines

Cigarette smoking causes approximately 30% of all cancer deaths in the U.S. It is responsible for 85% of lung cancer deaths. Snuff-dipping is an acknowledged cause of oral cavity cancer and the use of moist snuff in the U.S. has increased remarkably in recent years. In spite of advances in tobacco control and smoking cessation, there are still 48 million smokers in the U.S., and about 25% of the adult population smokes.

Tobacco-specific *N*-nitrosamines are formed from tobacco alkaloids during the curing and processing of tobacco products. Seven tobacco-specific *N*-nitrosamines have been identified in tobacco products. Two of these, 4-(methylnitro-samino)-1-(3-pyridyl)-butanone (NNK) and *N*-nitrosonornicotine (NNN), are present in substantial quantities and are strong carcinogens. NNK is a potent pulmonary carcinogen in rodents and also induces tumors of the pancreas, nasal mucosa, and liver. NNN causes tumors of the esophagus and nasal mucosa in rats and respiratory tract tumors in mice and hamsters. A mixture of NNK and NNN induces oral tumors in rats. Based on their carcinogenic activities, the extensive data on the occurrence of NNK and NNN in tobacco products, and on biochemical studies, these researchers hypothesize that these compounds play a significant role as causative factors in human cancers associated with tobacco use. Although there are parallels between NNK and NNN metabolism in rodents and humans that support this hypothesis, there are key aspects that must be explored further.

The overall theme of this research project is to evaluate the carcinogenic potential of NNK and NNN in humans exposed to tobacco products by performing mechanistic studies of NNK and NNN metabolism and adduct formation. Understanding the mechanisms by which tobacco smoke carcinogens cause cancer may lead to new insights on individual cancer susceptibility and development of innovative strategies to prevent tobacco-related cancers.

The specific aims of this project are:

- To investigate stereoselectivity in the metabolism of NNK and NNN by delineating differences in the formation and further metabolism of enantiomers of the major NNK metabolite 4-(methylnitrosamino)-1-(3-pyridyl)-1-butanol (NNAL), determining differences in the stereoselectivity of metabolic activation of NNK, and examining differences in the metabolic activation and carcinogenicity of NNN enantiomers.
- To investigate deoxyribonucleic acid (DNA) and protein pyridyloxo-butylation by NNK and NNN by elucidating the structures of the major adducts formed with DNA and hemoglobin.
- To investigate the metabolism of NNK and NNN in humans by determining levels of NNN metabolites in human urine, characterizing previously unknown NNN metabolites, and examining NNK metabolites in the urine of snuff-dippers to determine their persistence after cessation and their amounts as a function of dose.

Research Group

John Jalas, Graduate Student Researcher
Shana Sturla, Research Associate
Hansen Wong, Graduate Student Researcher

John H. Kersey, Principal Investigator

Gene Expression Profiles of Leukemia Cells

These researchers are using the Computational Genetics Laboratory to compare gene expression profiles of human leukemia cells that do or do not express an MLL fusion gene, eventually identifying target genes for further study. In addition, the project compares the gene expression profiles of bone marrow cells from leukemic mice bearing the MLL-AF9 fusion gene to the matched non-leukemic mice.

Research Group
Ashish Kumar, Research Associate

Jeffrey S. Miller, Principal Investigator

Development of Human Natural Killer Cells

This project uses the resources of the Computational Genetics Laboratory to investigate the development (differentiation) of human natural killer cells by using the Gene Array technique. The researchers are comparing the gene expression in the different groups of natural killer cells.

Research Group
Feng Xiao, Research Associate

Sharon E. Murphy, Principal Investigator

Nitrosamines and P450s

Nicotine and related nitrosamines comprise a class of environmental carcinogens that requires metabolic activation to exert its carcinogenic potential. Enzymes of the cytochrome P450 family are responsible for this activation. Minor differences in nitrosamine structure lead to activation by different cytochrome P450s. Cytochrome P450s are found in all organisms from bacteria to mammals, and over 500 carrier deoxyribonucleic acid sequences have been identified. Most P450s are membrane bound and only recently have the first three-dimensional structures of mammalian P450s been published.

These researchers are using molecular modeling to determine the amino acids in the active site of cytochrome P450 2A enzymes important in substrate specificity. The P450 2A enzymes are very good at metabolizing nitrosamines, and understanding more about how very small differences in amino acid sequence can change the substrate specificity can help in understanding more about nitrosamine carcinogenesis.

Research Group

Vytas Raulinaitus, Graduate Student Researcher
Linda von Weymarn, Graduate Student Researcher

Brian G. Van Ness, Principal Investigator

Cancer Transplant Biology and Therapy

These researchers are using the Computational Genetics Laboratory for their research into the genetic mechanisms of cancer transplant and therapy. This includes immunoglobin gene regulation, molecular analyses of myeloma, blood and marrow transplant stem cells, and minimal residual disease.

Research Group

Paula Croonquist, Graduate Student Researcher

Lynda B. M. Ellis, Principal Investigator

Bioinformatics Databases and Select Targets for Vertebrate Functional Genomics

This researcher focuses on developing bioinformatics tools that support the work of colleagues in the life sciences. One project is an innovative microbial biotechnology database on the World Wide Web, the University of Minnesota Biocatalysis/Biodegradation Database. Another project is the creation of bioinformatics databases and select targets for vertebrate functional genomics. A final project is the study of economic models for the support of the biological database infrastructure.

Collaborators

Larry Wackett, Faculty Collaborator
Stephen Ekker, Faculty Collaborator
Scott Fahrenkrug, Faculty Collaborator

William B. Gleason, Fellow

Applications of Advanced Computation and Digital Simulation to Problems of Biomedical Relevance

The Gleason group is continuing to explore parallel processing strategies of potential widespread utility in mass spectrometry. These include rapid "on-the-fly" analyses that allow for immediate identification of peptide analytes or, in the case of a failure to identify, immediate interactive modification of instrumental parameters for further experimentation. Such an application is particularly appropriate for testing on the Supercomputing Institute's Netfinity LINUX cluster, where the group can test their ideas and determine the appropriate number of processors to use for a given application. An example of the use of a "naïve" parallelization strategy is shown in the figure (next page). This indicates that a small laboratory LINUX cluster of perhaps eight processors (running at about 2 GHz) would be suitable for an "on the fly" application. Off-line analyses still remain of great importance, particularly those that involve large databases such as the ever-expanding genomic databases for humans as well as other species. Here, parallel processing using the Supercomputing Institute's high-performance computers with large memory and disk capabilities is attractive.

Of continuing interest to the group is the fibroblast growth factor (FGF) family of proteins, now numbering more than twenty distinct proteins, not counting the observed phenomenon of alternative splicing, which produces additional variants of each sequence. FGF family members have diverse biological roles ranging from control of neurite outgrowth in normal development to involvement in the wound-healing process. FGF members share a common property, i.e. they bind heparin, a sulfated polysaccharide best known for its anticoagulation properties. The group is interested in studying the interaction of proteins with sulfated carbohydrate polymers related to heparin. Although there are crystal structures available for some family members many important FGFs have

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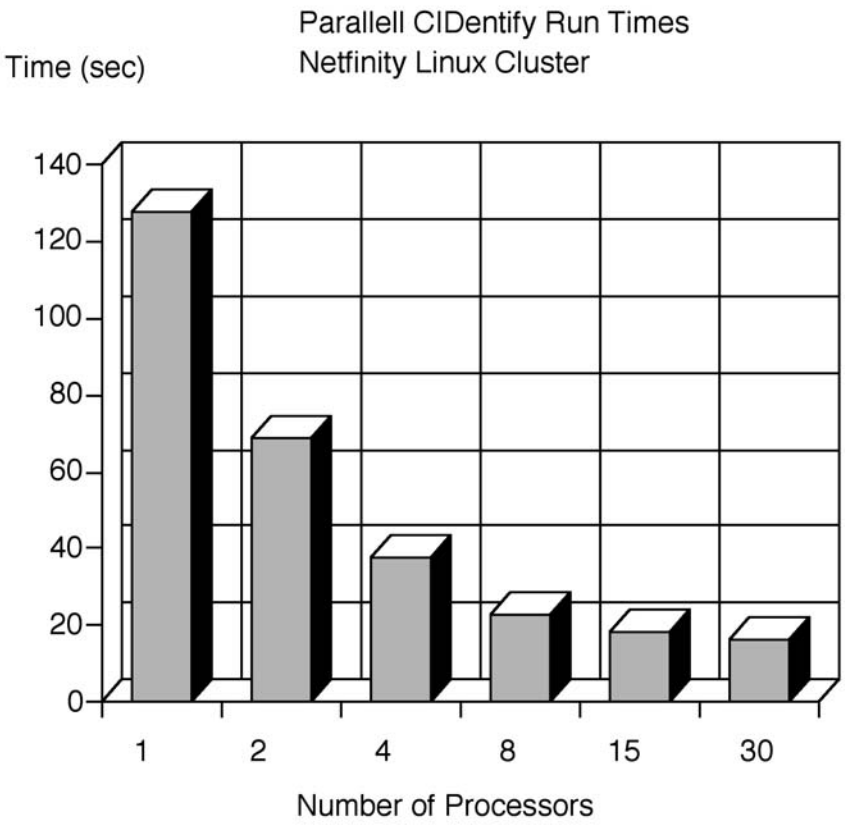
Research Group

Eric Eccleston, Research Associate
Eric R. Johnson, Supercomputing Institute Undergraduate Intern
William Ojala, Research Associate

William B. Gleason, Fellow



The non-redundant PIR file (a protein sequence file downloaded March 2, 2001) is used as a test database to search for five peptide sequences derived from MS. "Wall-clock" time drops from approximately 120 seconds on a single processor to approximately 20 seconds using 8 Pentium processors operating at 700 MHz.

available only sequence information. Thus these researchers are very interested in the use of homology modeling to construct three-dimensional models for FGFs using known crystal (or nuclear magnetic resonance) structures as templates. To that end they have constructed models for FGF-7 (whose three-dimensional structure is known) as well as FGF-13 for which no crystal structure is currently available.

The Gleason group continues to take a "tools approach" to their work in structural bioinformatics, dating back to the Protein Analysis Package (PAP) developed at the Supercomputing Institute in the early 90s. Thus Eric Johnson and Bill Gleason were invited to present a tutorial/workshop on the subject at the O'Reilly Bioinformatics meeting in early 2003. The highlight of the presentation was a series of movies made using the AMIRA package at the Supercomputing Institute that depicted a molecular dynamics simulation of heparin, an FGF family member, and an extensive illustration of the structural features of heparin important for its biological function.

Myron D. Gross, Principal Investigator

DNA Repair Genes and Breast Cancer

These researchers are working to identify human homologues of deoxyribonucleic acid (DNA) repair genes identified in other organisms. They then plan to use this information to further identify single nucleotide polymorphisms (SNPs) in these genes, and study the association of these SNPs with breast cancer. The researchers are using the Basic Sciences Computing Laboratory for this project.

Research Group
Bharat Thygarajan, Graduate Student Researcher

Franz Halberg, Associate Fellow

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. These researchers are developing a system for the chronobiologic analysis of cardiovascular records, with focus on disease prevention, but also addressing the question of the optimal scheduling of treatment when needed. Ambulatory devices are now used in different geographic locations that automatically monitor blood pressure and the electrocardiogram (ECG) for seven days at the outset. Chronobiologic analyses of such records serve first and foremost to assess how environmental factors affect human physiology, notably heart rate and blood pressure.

These researchers are using supercomputing resources to:

- Analyze beat-to-beat records for resolving chronobiologic and chaotic endpoints. A typical record consists of about 2,400,000 data points resampled at 0.25-second intervals over seven days.
- Automatically update reference standards as added data accumulate.
- Detect the earliest risk by means of chronome alterations.
- Follow up at-risk individuals longitudinally by means of control charts.

The researchers also recently found associations between endpoints of nonlinear dynamics computed on respiratory movement and electroencephalographic signals, which help the understanding of mechanisms underlying the coordination among physiological functions.

Towards this goal, the researchers are organizing existing records into databases. Reference values derived from these databases help detect any abnormality. A library of programs for such chronobiologic applications is being organized and integrated with the incorporation of graphic displays of the results.

The researchers have found that the vascular disease risks associated with reduced heart rate variability and with an elevated circadian ampli-

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Research Group and Collaborator
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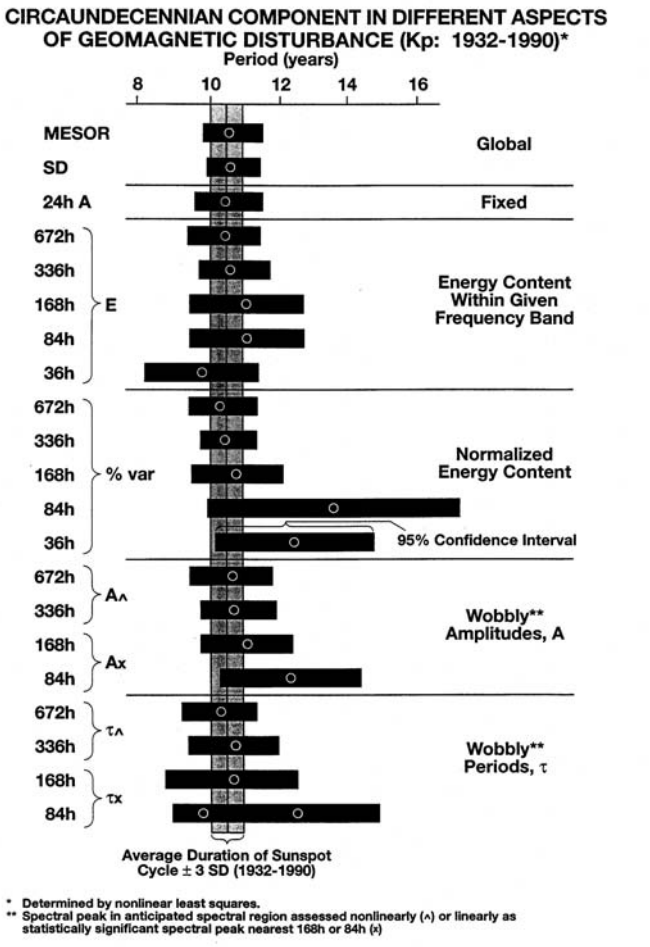
Franz Halberg, Associate Fellow

tude of blood pressure, documented in a number of trials, are mostly independent and additive. Also, the choice of treatment and its scheduling play important roles in normalizing altered dynamics of blood pressure and heart rate. Circadian hyper-amplitude-tension (CHAT), a condition defined by an excessive circadian amplitude of blood pressure (above the 95% prediction limit of healthy peers), occurs more frequently among patients with glucose intolerance. An odd timing of the circadian blood pressure rhythm in patients with non-insulin-dependent diabetes mellitus is associated with a reduced heart rate variability indicative of an impaired autonomic nervous system.

Analyses of magnetometer data over twenty-five months assessed time structures usually found in human physiology. In particular, the researchers assessed and quantified about-weekly components, which demonstrated the prominence of a natural component with a period shorter than seven days over the precise seven-day rhythm. This was also detected at Station A80 in Antarctica, about 600 km away from any civilization. The relative prominence of the man-made and natural components was used as an index to examine any change in human pollution in analyses of the global geomagnetic index. Maps of about 10.5-, 21-, and 50-year cycles in physical and physiological records are being prepared and interpreted in the light of two putative mechanisms underlying the influence of geomagnetic disturbances, acting via the heart and heart rate variability on the one hand, and via the pineal and melatonin on the other.



The global index of geomagnetic disturbance Kp is analyzed for the span from 1932 to 1990. Analyses are carried out over consecutive years to obtain estimates of the yearly mean value (MESOR) and standard deviation (SD) and of the amplitude, period, and power within given spectral ranges, around the month (solar rotation period), half-month, week, and half-week, as well as around 36 hours, as a control in a spectral region devoid of signals. The vertical band corresponds to the average duration of the sunspot cycle ±3 SDs for the same 59-year span. The horizontal bars correspond for each endpoint considered to the nonlinear estimate of the about 11-year cycle with the corresponding 95% confidence limits. Most point estimates fall within ±3 SDs of the average duration of the sunspot cycle. Of interest is the statistically significant modulation by the solar activity cycle of the circaseptan amplitude of Kp ($P = 0.031$), showing that this component is more prominent during years of descending than during years of ascending solar activity.

Kristin A. Hogquist, Principal Investigator

Peptide Induction of Positive Selection

Positive and negative selection are the critical forces that shape the T cell repertoire. This project addresses the molecular mechanisms of positive selection using a model system where defined peptide ligands can be used to preferentially induce one selection outcome or the other. These researchers use confocal microscopy and gene array technology to identify the molecules that are integral to the processes of positive and negative selection of T lymphocytes.

Research Group

Timothy Starr, Graduate Student Researcher

Amy P. N. Skubitz, Principal Investigator

Cell-Cell and Cell-Matrix Interactions

In ovarian carcinoma, cancer cells are shed from the surface of the ovary into the peritoneal or ascitic fluid. These cells may then adhere to the mesothelial cells and their associated extracellular matrix molecules that line the organs of the peritoneum. Subsequently, the ovarian carcinoma cells may migrate through the lining of mesothelial cells and underlying basement membrane to establish secondary growth sites. This multi-step process of adhesion, migration, and invasion eventually results in the death of the patient. These researchers are exploring the role of integrins and CD44 in the interaction between ovarian carcinoma and mesothelial cells, and are also investigating how ovarian cells that are shed into the ascitic fluid are kept in a nonadherent and/or noninvasive state. These studies represent an approach towards understanding the molecular mechanisms modulating the phenotypic behavior of carcinoma cells and may potentially aid in designing biopharmaceuticals for therapeutic use in cancer.

Research Group

Suzanne Grindle, Research Associate

Robert J. Bache, Principal Investigator
Yingjie Chen, Co-Principal Investigator

Myocardial Perfusion in the Hypertrophied Heart

The purpose of this study is to determine the factors that affect myocardial perfusion and energy metabolism in the hypertrophied heart. The researchers are using gene chips and computational software for gene chip analysis available in the Computational Genetics Laboratory.

Timothy W. Behrens, Principal Investigator

Discovery of Biomarkers for Rheumatic Diseases

The goal of this research project is to integrate a variety of cutting edge discovery technologies in order to discover novel biomarkers that will be clinically useful in one of the two major rheumatic diseases, rheumatoid arthritis and systemic lupus erythematosus. These technologies include broad gene expression profiling using deoxyribonucleic acid microarrays, combined with novel approaches to multi-parameter analysis of cell surface and soluble proteins relevant to inflammatory disease states.

Research Group

Emily Baechler, Research Associate
Sudha Balasubramanian, Research Associate
Karl Espe, Research Associate
Karis Hughes, Research Associate
Ward Ortman, Research Associate

Arkadiusz Z. Dudek, Principal Investigator

Microarray Analysis of Lung Cancer

Lung cancer is a leading cause of cancer morbidity and mortality. In 2002, its incidence has been estimated to be second only to prostate cancer in men and breast cancer in women. The clinical course and response to therapy of adenocarcinoma and squamous cell carcinoma of the lung may be very different. These differences may have origin in various changes in the expression of a number of genes.

This research project uses microarrays to analyze genes, discriminating normal lung tissues and adenocarcinoma and squamous cell carcinoma of the human lung. Ribonucleic acid (RNA) from all tissues was prepared and gene expression was determined at Gene Logic, Inc. (Gaithersburg, Maryland) using Affymetrix U95 arrays containing approximately 12,000 known genes and 48,000 expressed sequence tags (ESTs). The researchers are analyzing this data using the resources of the Computational Genetics Laboratory. Genes with at least four fold differences among the tissues and with p-value <0.001 for the fold difference were clustered by GeneData EXPRESSIONIST. Normal lung tissues, adenocarcinoma, and squamous cell carcinoma were well differentiated when these genes were clustered. Genes responsible for cell growth, RNA processing, and apoptosis inhibition were upregulated in adenocarcinoma. Squamous cell carcinoma showed higher expression of myc genes and genes responsible for cytoskeleton organization. Genes responsible for cell-cell adhesion, tumor suppression, components of peroxisome, and proteins involved in signaling pathways were downregulated in both adenocarcinoma and squamous cell carcinoma. Many genes differentially expressed in lung tissues were either ESTs or with not yet known functions. These changes in gene expression in adenocarcinoma and squamous cell carcinoma compared to normal lung tissues should help in understanding the biology of lung cancer, and may be useful in its diagnosis and treatment.

Research Group

Hemchandra Mahaseth, Research Associate

Patrick M. Gaffney, Principal Investigator

Gene Expression Profiling in Head and Neck Cancers

Cancer of the head and neck is a functionally, economically, and cosmetically devastating disease that accounts for approximately five percent of all cancers diagnosed in the United States. Although treatment with surgery, radiation therapy, or a combination of both can produce excellent results in early stage disease, only about one third of patients have highly confined lesions. The remaining two thirds of patients have local or regionally advanced disease. In spite of optimum local therapy, 50–60% of patients with advanced disease will subsequently develop local disease recurrence and 30% or more will develop distant metastatic disease. Standard chemotherapy in this patient group produces overall response rates of 30–50%, complete response rates of 5–27%, and a median survival of only four to six months.

Although characteristic morphologic features are similar among tumors arising from the same anatomic site, the presence of "molecular heterogeneity" is evident in the variety of genetic abnormalities described in head and neck cancer. These include activation of various oncogenes, tumor suppressor gene inactivation, and loss of heterozygosity at numerous chromosomal locations. The expression patterns of these and many other genes implicated in cancer development and progression, including many sequences of unknown function, will probably be important to understanding the variability in patient outcome experienced in the clinic.

In order to better understand the genes involved in head and neck cancer, these researchers have initiated a gene expression profiling study of squamous cell carcinoma tumors resected at surgery. Thirty-eight specimens have been subjected to microarray analysis using the Affymetrix U133 GeneChip system thus far and a correlation of gene expression data with clinical information is ongoing. The researchers are using the EXPRESSIONIST software package at the Computational Genetics Laboratory to further analyze and interpret the gene expression profiles.

Research Group

Matt Ginos, Research Associate

Jennifer L. Hall, Principal Investigator

Gene Expression Alterations

The goal of this research project is to determine gene expression alterations in the failing human heart in response to mechanical assistance support. The researchers are using the EXPRESSIONIST software package at the Computational Genetics Laboratory to array 200–250 paired heart samples over the next five years.

Research Group

Ami Mariash, Research Associate
David Fermin, Graduate Student Researcher
Suzanne Grindle, Research Associate

Robert P. Hebbell, Principal Investigator

Endothelial Cell Gene Expression as a Contributor to Clinical Phenotype in "Single Gene" Disorders

These researchers believe that inherited differences in vascular endothelial cell gene expression help define clinical phenotype in vascular disorders. An example is sickle cell anemia, a "single gene" disorder in which some children are at risk for stroke and others are not. Having developed the unique ability to obtain cultures of endothelial cells from a peripheral blood sample, these researchers are attempting a new experiment. They are taking endothelial cultures from patients with a defined phenotype (e.g., those with a stroke risk vs. those without a stroke risk) and examining patterns of endothelial gene expression. The researchers expect to find genes that contribute to phenotype. The analysis of the gene expression chip arrays is being done with the resources of the Computational Genetics Laboratory and the Basic Sciences Computing Laboratory.

Research Group

Aixiang Jiang, Research Associate

David T. Kiang, Principal Investigator

HCG Oligopeptide in Breast Cancer Prevention

Human chorionic gonadotropin (hCG) can prevent *N*-nitrosomethylurea carcinogen-induced rat mammary tumor. The mechanism of this process is still unclear. This project will use the microarray technique to probe this mechanism. Data analysis and interpretation are the crucial components of the project.

Richard A. King, Principal Investigator
Marshall I. Hertz, Co-Principal Investigator

Microarray Analysis of Gene Expression Patterns

Lung and heart-lung transplantation have become highly effective means of treatment for over 10,000 individuals worldwide with diseases not responsive to other medical and surgical therapy. Chronic rejection is the most significant limiting factor to long-term survival of lung transplant recipients; acute allograft rejection is a major cause of morbidity and is the most common risk factor identified for the development of chronic rejection. The overall goal of this project is to use microarrays to identify gene expression patterns in bronchoalveolar cells and peripheral blood mononuclear cells of lung transplant recipients with and without rejection. In doing so, these researchers aim to identify biomarkers for the prevention, prediction, and treatment of acute and chronic allograft rejection.

Research Group
Jeffrey D. Lande, Graduate Student Researcher

Kathy L. Moser, Principal Investigator

Gene Expression Profiling of Immune System Disorders

These researchers are using the resources of the Computational Genetics Laboratory for two closely related projects. The first project uses gene expression profiling to investigate Sjögren's Syndrome (SS), a chronic autoimmune disease that preferentially affects the lachrymal and salivary glands. Extraglandular features are also common and patients also exhibit a spectrum of clinical manifestations. The underlying etiology is poorly understood, but is likely to involve environmental and genetic factors interacting to cause dysregulation of immune responses that lead to both organ-specific and systemic autoimmune phenomena. These researchers have hypothesized that SS patients have characteristic gene expression profiles that may reflect underlying pathophysiologic processes. They are using microarray technologies to examine the expression of thousands of genes simultaneously in cells from SS patients. These data will be compared with gene expression profiles from age, gender, and race-matched controls. The researchers will also compare their results to similar data sets being compiled for systemic lupus erythematosus and rheumatoid arthritis in an attempt to characterize relationships between these three related autoimmune diseases. The results could identify genes with altered expression in SS, thus providing important new information that can be used to develop more effective diagnostic and therapeutic strategies for SS.

The second project investigates Antiphospholipid Syndrome (APS), a condition where the immune system mistakenly produces autoantibodies that bind to various phospholipids, resulting in clinical manifestations such as recurrent clotting, strokes, and spontaneous miscarriages. The cause probably involves both environmental and genetic factors, but only a small fraction of human genes have been examined for involvement in APS patients. These researchers are working to assess the activity of thousands of genes simultaneously. They hope to identify gene expression signatures that are specifically associated with APS. This could provide important new opportunities for designing more effective diagnostic tools and therapies for APS.

Research Group

Eshrat Emamian, Graduate Student Researcher
Martha Grandits, Research Associate
Carolyn Meyer, Research Associate

Gary M. Dunny, Principal Investigator

Modeling the Structure of the PrgZ Pheromone Binding Protein

The objective of this research is to use computer modeling to formulate the structure of the PrgZ protein of *Enterococcus faecalis*. This bacterial cell surface protein functions to bind the peptide sex pheromone cCF10 in order to initiate a bacterial mating response. The researchers are using a *Salmonella typhimurium* protein called OppA as a template for the modeling. This protein has a similar function, and its crystal structure has already been determined. PrgZ shares 40–50% of its amino acid sequence with OppA. The researchers are using the Basic Sciences Computing Laboratory for their modeling work.

Research Group

J. Michelle Antiporta, Graduate Student Researcher
Cathleen Earhart, Research Associate

David H. Sherman, Principal Investigator

Genomics of Antibiotic Biosynthesis in *Streptomyces Coelicolor*

The goal of this project is to develop a rational approach for metabolic engineering of secondary metabolite production in *Streptomyces coelicolor* using microbial genomic technologies. In this work, genome-wide microarray, green fluorescent protein (GFP)-based proteomic modeling, and Boolean modeling are employed to analyze two component regulators of secondary metabolism. Data are combined to obtain information on temporal, spatial, and conditional expression of key global and pathway-specific regulatory factors for four natural product biosynthetic pathways in this robust model microorganism. These pathways are actinorhodim, undecylprodigiosin, calcium dependent antibiotic, and methlenomycin. In order to establish the fundamental control architecture in these multi-step biosynthetic pathways, the prototype *absA* two-component regulatory system and 10 related two-component regulators are being investigated and their role in the circuitry of secondary metabolism defined. The results of this primary study will be used to probe the layers of control that will evolve from the initial analysis of the regulatory circuit. Use of high-throughput cloning of regulatory genes, construction, and phenotypic analysis of corresponding disruption mutants and temporal-spatial profiling of the resulting GFP-fusion proteins will provide important new information to develop a complete regulatory road map for control of antibiotic biosynthesis.

A new project uses structural and homology modeling to examine substrate binding in the mitomycin drug-binding protein MRD and a close structural homologue, FrbJ. The group is using molecular modeling to visualize the protein-substrate complex of MRD and then mutate the active site residues in the model to see how substrate binding is affected. They are also building a model of FrjB based on the crystal structure of MRD. This work will be extended by mutating the conserved active site residues in the model to determine which residues are critical for the binding of its substrate.

Research Group

Noelle Beyer, Graduate Student Researcher

Peter Southern, Principal Investigator

Human Organ Cultures and Microbial Infections at Epithelial Surfaces

A significant fraction of all human exposure to infectious microbial agents occurs at epithelial surfaces. To be as effective as possible, vaccines and other interventive strategies should establish potent barriers to prevent microbial infections' starting at epithelial surfaces. Systematic study of the cellular and molecular mechanisms that underlie transmission of microbial infections across epithelial surfaces will allow researchers to design and evaluate effective protective mechanisms.

These researchers have developed human organ culture protocols to analyze transmission and the initiation of microbial infections in experimental systems that are based entirely on human materials. Intact epithelial surfaces from tonsil, ectocervix, and endocervix have been infected by exposure to HIV (human immunodeficiency virus) to validate the overall feasibility of this approach. However, with a broader perspective, human organ culture systems can be utilized to develop a comprehensive understanding of the cellular and molecular mechanisms for mucosal transmission of a wide variety of human pathogens.

The researchers are now developing a multimicroscope approach to reconstruct infectious processes in biologically relevant tissues. They are using the resources of the Basic Sciences Computing Laboratory to explore the most effective methods to analyze confocal microscopy data relating to binding and penetration events at the surface of live tissue pieces exposed to viruses, bacteria, fungi, and protozoa.

Research Group

Diane Maher, Graduate Student Researcher

Bagrat Amirikian, Principal Investigator

Three-dimensional Lattice Model of the Motor Cortex: Emergence of Topologically Ordered Neuronal Structure With Coherent Properties

The long-term goal of this research project is to elucidate a relationship between the structure and function of fundamental distinct areas in the neocortex, in general, and the motor cortex, in particular, by a combination of theoretical methods with experimental approaches. The researchers are working to advance the understanding of whether and how the spatio-structural constraints on intrinsic connectivity affect the segregation of neurons into functional modules. They are working on a three-dimensional lattice model that allows for a fundamentally novel approach to studying directional operations performed in the motor cortex by providing means for explicit exploration of the link between the underlying local cortical structure and global collective properties of interacting cells that are substrates of this structure. This three-dimensional lattice model is heavily based on the accumulated knowledge of the neuroanatomy and neurophysiology of the motor cortex. The model will allow the researchers to bridge theoretical frameworks and experimental data in the domain of very large-scale simulations of networks of simplified neurons.

Recent work on this project has continued to focus on the use of neural network models to understand the processes underlying the brain's control of movement. The researchers have developed a parallelized learning algorithm that was used to optimize an artificial neural network for the task of translating neural signals generated by populations of cells in the motor cortex into meaningful movement commands. They have tested the parallelized learning algorithm against serial versions and have found that it significantly reduces the amount of time required for the artificial neural network to converge on a near-optimal solution.

The researchers have also begun construction of a large-scale model of a neural network with realistic connectivity. Supercomputing resources have been used to benchmark the processing times required for serial simulations of the network. The group's next task is to compare these results to those of a parallel version of the model, which is under development.

Research Group

Thomas Naselaris, Graduate Student Researcher

Aaron David Redish, Principal Investigator

Electrode Localization Through Reconstruction of Three-dimensional Patch/Matrix Anatomy From Two-dimensional Histological Slices

Striatal dysfunction has been implicated in a number of human diseases, including Parkinson's disease, Huntingon's disease, obsessive-compulsive disorder, and Tourette's syndrome. These researchers are studying the behavioral correlates of striatal cells in rats; that is, they record the firing of striatal neurons and ask what information is carried by those firing patterns. The recording technology consists of twelve individual electrodes, each capable of recording the separate spike trains of three to five cells. The striatum consists of a complex, interdigitated structure called *patch* and *matrix*. Although these two "components" consist of similar cell types (thus the recordings look similar from an electrical standpoint), they have very different input and output pathways (thus, they should process very different information). These two compartments are detectable using immunohistochemistry, staining thin-sliced (40 μm) sections for μ-opioid receptors. The researchers can also detect the positions of the electrodes were within these sections. However, they cannot tell which electrode corresponds to which marker.

In order to solve this problem, the researchers are using resources of the Basic Sciences Computing Laboratory to reconstruct the slices into a three-dimensional structure that will allow them to see the paths of all twelve electrodes directly and to see the three-dimensional structure of the patch/matrix. This will allow them to determine the locations recorded by each electrode and to measure the proportion of patch/matrix by each electrode. They will then be able to answer questions about the behavioral correlates of cells within patch and matrix.

Research Group

Deborah Bang, Graduate Student Researcher

Martin W. Wessendorf, Principal Investigator

Heterodimerization of Central Nervous System Receptors

Pairs of different g-protein coupled receptors have been reported to heterodimerize. By doing so, they should exist within a few nanometers of each other. If these receptors do in fact heterodimerize, it should be possible to use light microscopy to detect single structures in the central nervous system that are labeled for both receptors.

These researchers have been able to detect single structures at the limit of resolution by confocal microscopy (i.e., smaller than 0.3 μm) that are labeled for two different types of receptors. However, reception could in principle be improved by deconvolving the confocal images. The researchers are using the resources of the Basic Science Computing Laboratory to deconvolve such images. Obtaining higher resolution images will improve their ability to test which receptors, if any, may exist as heterodimers and to determine their distributions.

Research Group

Ming Gu, Graduate Student Researcher

George L. Wilcox, Fellow

Axonal Propagation of Impulses in Peripheral Afferents

This research project investigates the mechanisms of pain signaling and brain processing. Computational work in the laboratory involves the simulation of electrical excitability using molecular biological data and the analysis of time series data emanating from the brain. An object-oriented approach to incorporating molecular information allows the researchers to simulate phenotypes or the effects of genetic variations and mutations at the tissue and organ level. The response of cells and networks to sensory input and pharmaceutical interventions is also being explored.

The researchers are using a sound numerical time-integration scheme comprising a backward-differential time-stepper, a modified Newton nonlinear solver, and a preconditioned Krylov subspace iterative linear solver. They are simulating A-δ and C-fibers from rat peripheral nerve because of molecular information available from collaborators in the Ion Channel Group of the Center for Mechanisms of Human Toxicity at the University of Leicester. The tools developed in this project have a wide range of applicability, serving as a prototype for exploring disturbance in electrical activity in any excitable cell in the body. The use of molecular information in simulations is a novel approach to understanding cell function. Mutation information will allow researchers to examine various diseased states and the use of pharmaceutical agents will allow them to explore options in patient therapy.

Further research by this group involves the development of parallelized neural network-based algorithms for spectral and statistical analysis of spatio-temporal data from the new magnetocephalography unit recently installed at the Brain Sciences Center (VA) in Minneapolis. The aims of this work are to develop new strategies of multidimensional time-series analysis methods using novel means of audio-visualization. Several approaches involving neural networks, information theory, cost function minimization, techniques based on spectral and components analyses, and new experimental concepts being developed in auditory data display are being applied towards the audio-visualization and analyses of these complex multidimensional data. The heavy volume and high dimensionality of the time-series data acquired simultaneously from multiple recording channels make the audio-visualization problem ideally suited to a parallel computing environment.

Research Group and Collaborator

Apostolos Georgopoulos, Brain Sciences Center, Minneapolis Veterans Affairs Medical Center, Minneapolis, Minnesota

Pradyumna Upadrashta, Graduate Student Researcher

Anthony Varghese, Research Associate

Walter A. Hall, Principal Investigator

Analysis of Cranial Tumors

These researchers are using the resources of the Computational Genetics Laboratory to study the gene expression patterns of brain tumors. These tumors include aggressive tumors with metastatic potential and non-aggressive tumors. They are from both brain parenchymal and nonparenchymal sites. The researchers will compare them with each other and with other cancerous and non-cancerous tumors found in other parts of the body. The information will then be assessed using the results of magnetic resonance spectroscopic imaging that was taken as the time of tumor resection.

The researchers hope that the results of this study may lead to non-invasive ways of tracking the progression and growth of cranial tumors.

Research Group

Jesus A. Cabrera, Research Associate

Jack L. Lewis, Principal Investigator

The Effect of Mechanics Factors on the Degradation of Soft Tissues

Previous studies have shown that mechanics factors, such as the state of stress or strain, play an important role in cell death and subsequent functional degradation of the tissue in articular cartilage. The objective of this research is to identify, both qualitatively and quantitatively, the mechanical measures that are directly linked to tissue weakening and degradation. The research combines experimental and computational techniques.

Because of the complicated mechanical behavior of soft tissues, the researchers use numerical analysis (finite element analysis, FEA) to characterize the materials and extract the mechanics measures of interest. An extensive finite element method modeling and parametric study in the nonlinear FEA code ABAQUS and pre- and post-processing packages are also included. Because of the complexity and unique nature of the tissue materials, the general-purpose FEA code may not be sufficient to model some unique features observed in experiments, so user-interface programming is also included in this project.

Research Group

Hui Jin, Research Associate

Se-ho Park, Graduate Student Researcher

Jizhen Lin, Principal Investigator

Biology of Cochlear Hair Cells

Cochlear hair cells are specialized receptor cells for perception of sounds. A battery of transcription factors is involved in the development of hair cells and thousands of their related genes are expressed in this unique cell population, which acts in harmony to transform sound movements into perceivable electrosignals for the auditory cortex. Full knowledge of the genetic programs for cochlear development and a complete repertoire of gene expression in the cochlear hair cells is essential for understanding the generation of hair cells and the intricate and precise processes of hearing. Application of microarray, combined with carrier deoxyribonucleic acid (cDNA) subtraction, may lead to the discovery of genetic programs for hair cell regeneration and the repertoire of genes, known or novel, that direct hearing activity.

This project uses laser capture microdissection (LCM), a tool specifically designed to isolate single cells, to harvest pure cochlear duct and hair cells. After procuring target tissues or cells by LCM, the researchers isolate and amplify their full spectrum of messenger ribonucleic acid (transcriptome) using standard methods. They then profile the expression of transcription factors in cochlear ducts and their downstream molecules in hair cells. The first step is to use microarrays to determine the dynamic expression of transcription factors along the developmental path of hair cells. Next, cell culture systems are used to further characterize these transcription factors and their downstream molecules. Lastly, the researchers use cDNA extraction to identify novel transcription factor genes involved in hair cell development, followed by molecular cloning procedures for appreciation of their functions in hearing. Most, if not all, transcription factor genes involved in hair cell development should be identified through this comprehensive approach.

The central hypothesis of this study is that once the transcription factors for cochlear development and genes for hearing are appreciated, the molecular mechanisms for hair cell generation and hearing will be better understood. This will provide a foundation for rational design of innovative strategies for prevention and treatment of deafness, which affects almost thirty million Americans and costs the U.S. over $56 billion annually.

Research Group and Collaborators

Jasmine Duan, Graduate Student Researcher
Eric Javel, Faculty Collaborator
Vivek Kapur, Faculty Collaborator
Wei Pan, Faculty Collaborator
Vladimir Tsuprun, Research Associate
Jennifer Zhao, Graduate Student Researcher

Peter Santi, Principal Investigator

Computer Image Analysis of Macromolecular Arrays in the Cochlear Extracellular Matrix

The extracellular matrix is one of the basic constituents of the cochlea. It plays an important structural and mechanical role and is involved in transduction of sound-induced mechanical stimuli into electrical signals. Structural abnormalities of the matrix may lead to different types of hearing disorders. The overall goal of this project is to study the structure of symmetric macromolecular arrays in the cochlea. The project contains two specific aims:

- To determine the ultrastructure of the cochlear extracellular matrix. Supramolecular organization of collagen, fibronectin, tenascin, and other molecules may provide a foundation upon which micromechanical models of the cochlea can be constructed. The researchers are focusing on the ultrastructure of proteoglycans arrays in different types of cochlear basement membranes.
- To determine the structure of the outer hair cell stereocilia links. The structure of periodically arranged side links, rotationally distributed "attachment links" and helical organization of the tip-links are being investigated to find a relationship between the structure and role of these symmetric arrays. The tip-links play an important role in mechano-electrical transduction of the sound waves, and a substantial part of this project includes the study of its helical structure found recently in these links.

Research Group

Vladimir Tsuprun, Research Associate

Bruce R. Blazar, Principal Investigator
Angela Panoskaltsis-Mortari, Co-Principal Investigator

Identification of Gene Expression of Type II Pneumocytes

Keratinocyte growth factor (KGF) is a potent mediator of epithelial cell proliferation, as well as a growth factor for type II pneumocytes. KGF has also demonstrated cytoprotective properties against chemotherapy and radiation-induced injury. These researchers have previously shown that KGF administration prior to chemotherapy-induced injury ameliorates graft-versus-host disease and idiopathic pneumonia syndrome in a murine allogeneic bone marrow transplantation model. Investigations into the role of KGF in the lung have observed increased lung surfactant levels, increased alveolar fluid clearance, and decreased hyperoxic injury of type II pneumocytes. In order to further evaluate the mechanism of KGF-induced protection of the lung, these researchers are performing microarray analysis on KGF receptor-positive lung cells. To do this, they use laser capture microdissection to collect KGF receptor positive cells from innumohistochemically stained mouse lungs after 24 and 73 hours of systemic KGF administration. Then, ribonucleic acid (RNA) is isolated from the captured cells and amplified through two subsequent rounds of *in vitro* transcription. The resulting RNA is then applied to an Affymetrix GeneChip for expression analysis.

The researchers hypothesize that they will find increases in expression of genes involved in deoxyribonucleic acid repair, surfactant production, alveolar fluid clearance, and other protective processes. They think they may also see a decrease in expression of apoptotic genes. After characterization of genes important for protection by KGF, the researchers may be able to investigate possible avenues for increasing the therapeutic benefit of KGF treatment.

Research Group

John Hermanson, Graduate Student Researcher

Michael Mauer, Principal Investigator

Microarray Studies of Skin Fibroblasts in Type 1 Diabetes

Diabetic nephtopathy (DN) is the leading cause of kidney failure and was responsible for 44% of all the new cases of kidney failure in the U.S. in 2001. These researchers are studying cultured skin fibroblast (SF) and renal proximal tubal epithelial cells (PTEC) from type 1 diabetic patients in order to better understand the differences in behavior of these in patients with and without DN. They are testing the hypothesis that there are inherent cellular differences between type 1 diabetic patients with or without DN, and that these differences are genetically determined and are associated with altered SF and/or PTEC gene expression.

There is accumulating evidence that genetic factors not associated with the risk of type 1 diabetes convey risk or protection from DN. The evidence is originally derived from the observation of familial clustering of DN risk. Type 1 diabetic siblings of DN patients have a five-fold higher prevalence of DN than do type 1 siblings of patients without DN. Studies also demonstrate concordance for the severity and patterns of glomerular lesions in type 1 sibling pairs, even after factoring for metabolic control, duration of diabetes, and other factors. However, the genes that may be involved in the pathogenesis of DN are unknown.

Several research groups are exploring the specific genes responsible for the onset or progression of DN, but the single candidate gene has approach has been inconclusive. One approach is to study cells *in vitro*, which, after several passages in tissue cultures, can be assumed to better reflect intrinsic rather than environmental factors. The goal of these researchers is to use microarray techniques to test for gene expression differences in total ribonucleic acid isolated from SF and PTEC from type 1 diabetic patients that have been structurally and functionally polarized into two groups: one a "fast-track" group (high risk of DN) and one a "slow-track" group (low risk of DN).

Research Group and Collaborator

Luiza Caramori, Research Associate
Shirley Chang, Research Associate
Chunmei Huang, Research Associate
Yongdae Kim, Faculty Collaborator
Paul Walker, Research Associate

Stanley A. Thayer, Principal Investigator

Role of Mitochondria and Ca^{2+} in Glutamate-Induced Neurotoxicity

Glutamate-induced neurotoxicity may underlie the mechanisms of many neurological diseases. Overstimulation of glutamate receptors results in Ca^{2+} overloading and mitochondrial dysfunction. This project investigated whether the interactions between Ca^{2+} and mitochondria contribute to glutamate-induced neurotoxicity. Using the resources of the Basic Sciences Computing Laboratory, the researchers employed a variety of techniques to measure intracellular and intra-mitochondrial Ca^{2+} concentrations, neuronal inability, mitochondrial function, and biochemical events induced by mitochondrial uptake of Ca^{2+}. Pharmacological agents and molecular engineering approaches were used to dissect the molecular pathways involved and the targets for intervention.

Research Group
Guang Jian Wang, Research Associate

Jürgen F. Fohlmeister, Principal Investigator

Modeling of Complex Systems

This researcher is involved in three projects using the modeling capabilities of the Basic Sciences Computing Laboratory. Two of these projects investigate aspects of neural excitation, and the third investigates the behavior of proto-continents.

The first project investigates the role of membrane capacitance in neural excitation. Although membrane capacitance (1 mF/cm^2) was accurately measured about two decades prior to the first delineation of the ionic currents responsible for the nerve impulse (the Hodgkin-Huxley model), capacitance of the neural membrane has generally been regarded as an unavoidable and unimportant linear path in parallel with the critical sodium, calcium, and potassium currents (Na-, Ca-, and K-currents). More recently, however, it has become important to model impulse encoding in neurons of the central nervous system with non-uniform channel density distributions, for which the membrane capacitance can introduce unexpected excitation phenomena. This research project has shown that these phenomena are of two kinds, which are related to the charge-storage function of capacitance. In the space-clamped mode, capacitance can act as a battery; stimulus current can charge the membrane capacitance, which is capable of holding it voltage under certain circumstances. This occurs when regions of low channel density are present in the neural morphology; the local low charge leakage can control the dynamic range of impulse frequency generation. This is found specifically in retinal ganglion cells (as well as hippocampal neurons), where the distribution and density of channels on the dendrites becomes an important factor in impulse encoding, even when the dendrites themselves are incapable of supporting impulses on their membrane. Other specialized neural regions, specifically the impulse "trigger zone," which operates with the highest

Jürgen F. Fohlmeister, Principal Investigator

electrically gated channel densities, also interact with their neighboring membranes to determine the rate of impulses on their membrane.

Another project involves neural excitation as a function of temperature in the squid axon membrane. Although the Hodgkin-Huxley model for the squid axon membrane is incapable of generating nerve impulses at mammalian temperatures, the mathematical structure of the Hodgkin-Huxley equations has nevertheless been the basis for their simulation throughout the last half-century at all physiological temperatures. This has been achieved by ad hoc adjustments to the equations. This research shows that the primary reason for the mammalian temperature failure of the Hodgkin-Huxley model lies in the magnitude of that model's gating kinetic rate constants in the presence of membrane capacitance; in the absence of the capacitance, the model will generate impulses at all temperatures. Applying the Q_{10} factor of three to the temperature dependence of all rate constants narrows the impulse from 2.5 ms (6.3 °C) to 0.6 ms (38 °C) in the absence of the capacitative current; on the other hand, the impulse collapses for the same (and lesser) temperature shifts in the presence of capacitance. Phase space analysis shows that the repolarizing K-current overtakes the normally faster regenerative Na-current, because the rapid rate-of-rise of the Na-current is compromised by the necessarily accompanying large capacitative current, which is proportional to the rate-of-rise. The slower-recovering K-current is associated with a smaller time-rate of voltage change, and is therefore less affected by capacitative current. This research project has shown that phase space analysis offers the necessary adjustments to voltage-clamp data, which are typically contaminates by artifacts due to the difficulty of achieving the necessary space-clamp, effects that are most pronounced in simulations involving large time-rates of change.

The final project created a "sticky" model that simulates the primordial accreting process of continents and their associated tectonic plates. Buoyant "flakes" of hard materials are assumed to be persistently and randomly generated at isolated convective up-welling centers of the rocky Earth (mantle), and are driven horizontally and radially away from the up-welling centers (hotspots) on the upper surface of convection cells. These flakes accumulate and represent the growth of the continents and associated tectonic plates.

David G. Levitt, Associate Fellow

Protein Structure Determination and Development of Software for Automated Fitting of X-ray Crystallographic Electron Density Maps

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 selenomethione multi-wavelength anomalous dispersion phasing techniques made the generation of high-resolution electron density maps a routine procedure. The most time-consuming step is the building of the initial protein structure into the electron density map. This procedure takes several months of a skilled investigator's time working at a high-quality graphics station.

The goal of this project was to develop a program to automate this procedure by allowing a researcher to input the electron density map and the amino acid sequence to the computer, which would then return an accurate initial structure that could be used as input to refinement programs. The program is nearly complete and is being tested at several laboratories. It is now possible to automatically fit nearly all the secondary structure. The next step is to extend these secondary structures into the loop regions. It should then be 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 was developed for this project.

Research Group
Timothy A. Anderson, Research Associate

Esam E. El-Fakahany, Principal Investigator

Modeling the M1 Muscarinic Acetylcholine Receptor

These researchers have extensively used Supercomputing Institute resources to determine how drugs of potential therapeutic applications interact with their target sites. Specifically, they used a three-dimensional computer model of receptor structure to investigate the receptor elements responsible for drug binding. This approach has been applied to their studies of the interaction of the novel compound xanomeline with acetylcholine muscarinic receptors. Xanomeline has a potential to serve as a prototype of a drug to be used for treatment of memory deficits in Alzheimer's disease. Computer modeling studies using the Basic Science Computing Laboratory have enabled the researchers to predict the sites of interaction. This information will be substantiated by making changes in the receptor or the xanomeline molecule.

Research Group and Collaborators
David M. Ferguson, Faculty Collaborator
Marianne Grant, Research Associate
Fei-Fan Guo, Research Associate
David Saffen, Faculty Collaborator

Rolf Grütter, Principal Investigator

Analyzing Spectra Using One- and Two-dimensional Methods

This research project focuses on analyzing one- and two-dimensional nuclear magnetic resonance (NMR) spectra acquired using high-field NMR spectrometers on *in vitro* and *in vivo* data. Specifically, the research component is focused on detailing the information content of such spectra, spectral simulations, and the fitting of systems of 25 differential equations to time courses measured *in vivo*. The goal of this research is to pinpoint the modeling constraints that are necessary to determine the rate of neurotransmission in the brain *in vivo* and to measure approximately 20 neurochemicals simultaneously *in vivo* from very small volumes. The final goal of this research is to provide fundamental insights into the biochemical regulation of the brain and to understand the regulation of brain metabolism during hypoglycemia, which has been identified as the major roadblock in the treatment of diabetes.

Research Group
Gulin Oz, Research Associate
Ivan Tkac, Research Associate

Peter S. Dahlberg, Principal Investigator

Gene Expression in Esophageal Adenocarcinoma

This researcher is using the Computational Genetics Laboratory to study gene expression in esophageal adenocarcinoma using microarray and other molecular biology techniques. The project's goal is to develop rational therapies based on the control of abnormally expressed genes.

David L. Dunn, Principal Investigator
Karen R. Wasiluk, Co-Principal Investigator

Protection During Gram-negative Bacterial Sepsis

Gram-negative bacterial sepsis and shock continue to be significant causes of morbidity and mortality for surgical patients. Despite improvements in antibiotic therapy and intensive care, mortality associated with this condition remains at approximately 40%. Increasing evidence indicates that the lipid A portion of the lipopolysaccharide (LPS, endotoxin), an integral portion of the gram-negative bacterial membrane, interacts with a variety of host defenses to cause the release of cytokine mediators of sepsis, such as tumor necrosis factor-alpha, interleukin-1-beta, interleukin-6, and interleukin-8.

The objective of this project is to develop, characterize, and test LPS antagonists. There are two specific aims. The first is to develop and characterize *in vitro* the inhibitory activity of a large number of LPS antagonists. The second is to examine the protective capacity and to determine the mechanism(s) of action of each of these LPS antagonists *in vivo* in animal models of experimental gram-negative bacterial sepsis and endotoxemia. In addition to survival, the researchers are quantifying the neutralization and clearance of LPS, bacterial activity and bacterial clearance, and cytokine transcription, translation, and secretion in the local tissue milieu and the systemic circulation. The researchers compare and contrast the *in vitro* and *in vivo* results obtained from testing each type of LPS antagonist. Comparisons at the molecular level are being undertaken using sequencing and cloning techniques, to identify those critical regions of the molecule that are responsible for anti-LPS activity. This information will be used to delineate the molecular basis of endotoxin antagonism and to develop additional potent LPS antagonists.

Research Group
Suzanne Grindle, Research Associate

Kristen J. Gillingham, Principal Investigator

Random Assignment of Treatments in Solid Organ Transplant Research

Randomized clinical trials are often conducted in solid organ transplant research. Currently, such trials involve comparisons of various new immunosuppressive drugs to standard therapies studying the effectiveness of steroid withdrawal at various times post-transplant compared to usual steroid dosing, comparison of different prophylactic treatments to prevent infection post-transplant, and comparison of various anti-rejection treatments.

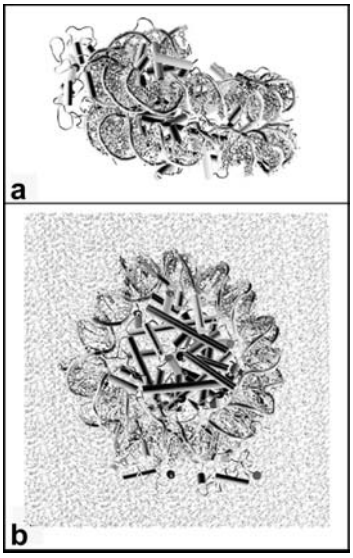
To implement the random assignment of treatments to patients in various kidney-transplant studies, this researcher has written a computer program in FORTRAN 77. This program, which is run on the supercomputers, provides individual randomization cards that are sealed in envelopes and "pulled" at the time a new patient enters a particular study. The program also provides a master list of treatment assignments for each study.

Lester F. Harris, Principal Investigator
Leonard S. Schultz, Co-Principal Investigator

Dynamic Simulations of Solvated Protein-DNA Complexes

These researchers are conducting experiments investigating the mechanism(s) of a genetic switch controlled by deoxyribonucleic acid (DNA) regulatory proteins. They are interested in steroid hormone receptor protein interaction with DNA in the pathogenesis of breast cancer. The researchers have previously reported on a mechanism describing how these DNA regulatory proteins recognize and bind to their specific sites on DNA. They are conducting Particle Mesh Ewald (PME) periodic boundary molecular dynamics simulations in solvent to investigate hydrogen bonding, van der Waals, and electrostatic interactions between amino acids of the of the DNA regulatory proteins and nucleotides of their cognate DNA biding sites. They have constructed separate large models of the 434 cI repressor and Cro proteins in complex with all three of the operators—OR1, OR2, and OR3—involved in regulation of a genetic switch. The models will allow the researchers to complete their study of the prokaryotic genetic switch regulating lytic/lysogeny expression in the 434 bacteriophage.

Using a high-resolution crystal structure of a nucleosome core particle of chromatin, the researchers have developed an exact nucleosome model of the 5′ long terminal repeat nucleotide sequence upstream of the mouse mammary tumor virus genome. This genome contains well-characterized DNA binding sites for steroid hormone receptor proteins. The model will allow the researchers to study eukaryotic regulatory elements in their natural context to develop a better understanding of the requirements for controlling expression of transfected genes.



a. A computer model of one glucorticoid receptor dimer in complex with a glucorticoid response element from the mouse mammary tumor virus 5′ long terminal repeat nucleosome DNA in a supercoiled conformation. b. The complex viewed along the DNA nucleosome axis shown in a water box for PME periodic boundary solvated molecular dynamics simulations.

The researchers have also constructed a model of the androgen receptor protein in complex with its cognate DNA binding site. This model will aid in the study of wetwork experiments in prostate cancer research.

Finally, the researchers are computing the PME periodic boundary solvated dynamic simulations on several other steroid receptor/DNA complexes. These studies include DNA-containing various hormone response elements (cognate and non-cognate) in complex with most members of the steroid receptor superfamily of proteins, particularly the estrogen, glucocorticoid, retinoic acid, and progesterone receptors.

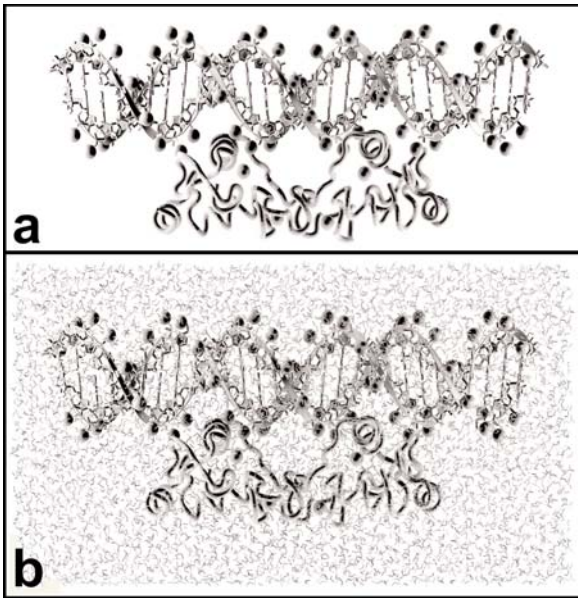
Continued on next page

Research Group

Pamela D. Popken-Harris, Research Associate
Michael Sullivan, Research Associate

Lester F. Harris, Principal Investigator
Leonard S. Schultz, Co-Principal Investigator

a. A ribbon structure of the androgen receptor protein dimer in complex with a 29 bp DNA sequence containing an androgen response element. b. The complex shown with a water box for PME periodic boundary solvated molecular dynamics simulations.



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 quantify 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 analysis—that is, for the first time we have a technique allowing a glimpse at the richness of structures that create the biologic signal. Further, despite the apparent system complexity, a dynamical analysis can reveal a series of simple rules that govern the system's behavior.

This study examines the electromyographic (EMG) signal present in the urethral striated muscle during bladder function.

Daniel A. Vallera, Principal Investigator

Antibody Modeling

This research group is synthesizing antibody fragments with the goal of making them usable in humans. They are using the Basic Sciences Computing Laboratory for computer modeling that will help the researchers optimize the fragments' binding ability.

Research Group

Xioax Feng, Graduate Student Researcher
Ni Jin, Graduate Student Researcher
David Kuroki, Research Associate
Yangyn Shu, Research Associate
Deborah Todhunter, Research Associate

Catherine M. Verfaillie, Principal Investigator

Stem Cell Research

The objective of this project is to study stem cell behavior, including proliferation, differentiation, and possibly "de-differentiation" to further the understanding of the potential of stem cells to improve human and animal health. This involves basis research into genetics and genomics, developmental biology, cell biology, and the physiology of stem cells and their differentiated progeny. The researchers are using the resources of the Computational Genetics Laboratory for this project.

Research Group

Craig Eckfeldt, Research Associate
Todd Lenvik, Research Associate
Beatriz Pelacho, Research Associate
Huilin Qi, Research Associate
Stephanie Salesse, Research Associate
Robert Schwartz, Graduate Student Researcher
Fernando Ulloa, Research Associate

James R. Fricton, Principal Investigator

National Institute of Dental and Craniofacial Research's Implant Registry and Repository

Temporomandibular joint disorders (TMJs) are common disorders causing facial pain, headaches, and clicking, locking, and diminished functioning in the jaw. In some cases, there is degeneration of the temporomandibular joint structure (bone and articular cartilage) leading to pain, dysfunction, and destructive changes in the joint. TMJ implants have been used with surgery to treat these conditions. Further research is needed to explain the diverse outcomes associated with TMJ patients and to discover what characteristics of TMJ implants are best tolerated and most successful in these patients.

This project will develop a nationally recognized research registry and repository that is designed to collect clinical information and biological specimens on patients with TMJ disorders throughout the United States. This will stimulate more research in TMJ disorders and advance the understanding and success of treatment of patients with this painful condition.

Research Group and Collaborators

Patricia Carlson, Research Associate
Nancy Hardie, Research Associate
Wenjun Kang, Research Associate
Lois Kehl, Faculty Collaborator
John Look, Research Associate
Sandra Myers, Faculty Collaborator
James Swift, Faculty Collaborator

Paul J. Jardine, Principal Investigator
Dwight L. Anderson, Co-Principal Investigator

Structure and Assembly of Bacteriophage Phi29

These researchers are working on the assembly and maturation of the bacterial virus phi29. Ongoing efforts are to determine the structure and function of various components of the molecular machine responsible for packing the viral deoxyribonucleic acid (DNA) genome into a preformed protein shell, or prohead. A crucial component of these efforts is the production of cryo-electron microscopic (cryo-EM) reconstructions. Much of these researchers' previous work has made use of expertise at other institutions. In order to enhance the quality of their efforts, these researchers are developing their own expertise in impact reconstruction. They are using software available in the Basic Sciences Computing Laboratory to undertake image reconstruction of a variety of components of the phi29 virus.

The main goals of this project are to improve the resolution of structures currently under investigation, and to begin new work on the study of structural symmetry mismatches in the components of the molecular machine.

Research Group

Lan Zhou, Undergraduate Student Researcher

Patrick W. Mantyh, Principal Investigator

Molecular Mechanisms of Bone Cancer Pain

The goal of this project is to gain a better understanding of the factors that generate and maintain bone cancer pain due to a mixed tumor (i.e., one that induces both bone destruction and formation). While the focus is on sensory and sympathetic neurons, the researchers are also examining how peripheral factors such as tumor growth, bone destruction, and sympathetic neurons excite or modulate sensory neurons and thus contribute to bone cancer pain. Similarly, the study examines how inputs from sensory fibers that innervate the tumor-bearing rat bone alter the cellular and neurochemical characteristics of the spinal cord and dorsal column nuclei and thus should contribute to central sensitization. These experiments should also provide insight into non-osseous types of cancer pain and aid in the development of novel strategies for controlling cancer pain in humans.

Research Group
David Mach, Graduate Student Researcher

Peter C. Raynor, Principal Investigator

Modeling of Airborne Particle Filtration

Fibrous filters are important tools for controlling exposures to potentially hazardous particles. New synthetic fibers with irregular cross-sectional shapes may improve filter performance beyond the capabilities of filters made with conventional fibers. The objective of this research project is to determine how much fibers with irregular cross sections can improve filter performance. The specific aims of the project are to:

- Develop flow fields for air moving past two-dimensional arrays of irregularly shaped filter fibers.
- Model the movement of particles through the flow fields.
- Calculate the efficiency of particle collection by fibers.

This work is being done using FIDAP computational fluid dynamics software on the supercomputers. This research will provide the first analysis of the possible advantages of using irregularly shaped fibers in filters. With this new information, filter manufacturers may be able to produce filters that can protect people better than is possible now.

Research Group
Seung Won Kim, Graduate Student Researcher
Ji Young Park, Graduate Student Researcher

William A. Toscano, Principal Investigator

Models of the Estrogen Activity of Bisphenol A Analogs

Bisphenol A (BPA) is a monomer constituent of epoxy and polycarbonate resins employed widely in consumer products. Many studies have shown that BPA is a weak estrogen receptor (ER) agonist with endocrine-disrupting potential in exposed organisms. These researchers have developed a series of quantitative structure activity relationship (QSAR) models generated to describe the *in vitro* estrogen activity (ER binding, reporter gene induction, MCF-7 proliferation) of 21 BPA analogs. The estrogen activity within this set ranged over four orders of magnitude with BPA displaying intermediate activity.

Research Group and Collaborator

Kelly P. Coleman, Graduate Student Researcher
Thomas Wiese, Department of Environmental Health Sciences, Tulane University School of Public Health and Tropical Medicine, New Orleans, Louisiana

The objectives of this project included both evaluating the ability of QSAR methods to describe the estrogen activities of the BPA analogs as well as characterizing the specific structural features responsible for this activity. Comparative molecular field analysis, comparative molecular similarity indices, hologram QSAR, and QSAR models using Molconn-Z connectivity, shape, and information indices were generated using the program SYBYL 6.8. Bisphenols with optimal estrogen activity contain two unencumbered phenolic groups in the *para* orientation as well as multiple alkyl substituents extending from the carbon-linking phenolic rings. Furthermore, the data suggest that it may be possible to use these structure-activity relationships to develop bisphenols with reduced hormone activity that maintain utility as polymer components.

James S. Pankow, Principal Investigator
Michael B. Miller, Co-Principal Investigator

Genetic Epidemiology of Cardiovascular Disease and Associated Risk Factors

This research project seeks to detect, localize, and characterize genes involved in the development of cardiovascular disease (CVD) and its associated risk factors (e.g., diabetes, high blood pressure, elevated blood cholesterol). Recent technological advances in molecular biology and genetics have provided new opportunities to explore the genetic architecture of complex diseases and traits such as CVD. However, genetic epidemiological research on such traits requires data on thousands of individuals, hundreds of genetic markers, and complex statistical models that are computationally demanding. Supercomputing resources are used to construct models with high order gene-gene or gene-environment interactions that cannot be practically evaluated otherwise, and to conduct simulation experiments.

Research Group and Collaborator

Donna K. Arnett, Faculty Collaborator
Sue Bielinski, Graduate Student Researcher
Projjwal Ghosh, Graduate Student Researcher
Karen Green, Graduate Student Researcher
Joanlise Leon, Graduate Student Researcher
Amy Lynch, Graduate Student Researcher
James Peacock, Research Associate
Laura Rasmussen, Graduate Student Researcher
Richard Sherva, Graduate Student Researcher
Weihong Tang, Research Associate
Kim Weis, Research Associate

Mayo Medical School

Department of Pharmacology

Yuan-Ping Pang, Principal Investigator

In Silico Drug Design

The focus of this research is the development and application of computational (*in silico*) methods for reliable determination of novel pharmaceutical drug leads. Viable drug candidates are predicted through the virtual screening of a database of millions of unique chemical structures against a target enzyme. Computationally identified leads are tested experimentally and optimized using combinatorial chemistry and medicinal chemistry.

In silico (virtual) screening studies are being performing using the researchers' advanced docking program, EUDOC. This program permits molecular docking studies with metalloproteins and uses "spatial-decomposition" to achieve 100% parallelism. A Mayo in-house database called CHEMIX that consists of about 2.5 million druggable molecules facilitates virtual screening of drug targets. The researchers plan to increase the reliability of docking studies by increasing the number of conformations stored per molecule in the database. This is done by obtaining CM2 atomic charges for all molecules and by taking into account the change in free energy of solvation due to receptor-ligand complexation. A goal for the virtual screening efforts is to identify better second-generation farnesyltransferase inhibitors as potential cancer drugs.

In addition, this group is studying the dynamic structure of the active site of cofactor-independent phosphoglycerate mutase using a lengthy molecular dynamics simulation. The characterization of this active site will allow for the future *in silico* screening of this target in the search for novel antibacterial agents, computational study of Sin3-mediated transcriptional repression, and BIR3 inhibitor design.

Research Group

Min He, Research Associate
Ganesh Kumar, Research Associate
Kevin J. Lagenwalter, Research Associate
Isidro Merino, Research Associate
James D. Xidos, Research Associate

Metropolitan State University

Department of Information and Computer Sciences

Jigang Liu, Principal Investigator

Performance Evaluation of Parallel Computational Geometry Algorithms

The goal of this project is to create an experimental environment for analyzing and evaluating the performance of parallel computational geometry algorithms. The environment has three major components: a data-acquiring system, a communication system, and a computation system. The data-acquiring system will be established using graphical user interface technology so that the user can freely define the scenarios for testing and evaluation purposes. The communication system is based on the UNIX PC mechanism using the TCP/IP protocol and works as a connection between the data acquiring and computation systems. The computation system is dedicated to the implementation of the existing and newly developed parallel computational geometry algorithms on the IBM SP supercomputer.

Minnesota State University–Mankato

Department of Management

Rakesh Kawatra, Principal Investigator

Multiperiod Minimal Spanning Tree Problem: Formulation and Solution Methods

The Multiperiod Minimal Spanning Tree problem consists of scheduling the installation of links in a network so as to connect a set of nodes to a central node with minimal present value of expenditures. Some of the nodes in the network are active at the beginning of the planning horizon while others are activated over time. The problem was formulated as an integer-programming problem. This project uses a Lagrangian-based heuristic to solve the integer programming formulation of the network problem. Lower bounds found as a byproduct of the solution procedure are used to estimate the quality of the solution given by the heuristic. Experimental results over a wide range of problem structures show that the Lagrangian based heuristic method yields verifiably good results.

A new research project uses the Lagrangian based heuristic to solve the problem of the hop constrained min-sum arborescence with outage costs. This problem consists of selecting links in a network so as to connect a set of terminal nodes $N = \{2, 3,.....n\}$ to a central node with minimal total link cost such that:

- Each terminal node j has exactly one entering link.
- For each terminal node j, a unique path from the central node to j exists.
- For each terminal node j the number of links between the central node and j is limited to a predefined number h_j.
- Each terminal node has an associated outage cost, which is the economic cost incurred by the network user whenever that node is disabled due to failure of a link.

The size of this problem and the computing speed required to solve it make the use of the supercomputers necessary.

St. Cloud State University

Daniel D. Gregory, Principal Investigator

G3 Calculations on C_2H_6SO Isomers

This project focuses on determining the G3 energetics for three isomers of C_2H_6SO and is part of a larger effort focused on the development of vicinal disulfoxide energetics. The G3 energy differences between the three isomers will be compared with those calculated at different basis sets and methods with the hopes of finding a less rigorous method and basis set that can be applied to larger systems. All the other computations have been completed, and this researcher is using supercomputing resources to perform the G3 calculations.

Collaborator
William S. Jenks, Department of Chemistry, Iowa State University

Andrew Allen Anda, Principal Investigator

Exploring High-Performance Computing With Parallel Matrix Multiplication

This project is intended to explore high performance computing using the supercomputers for parallel matrix multiplications. These researchers have recently changed serial codes into parallel codes. The codes are used to multiply to matrices with different methods, such as the Cannon method and the blocking method. The researchers are also planning to use BLACS and SCALAPACK function calls.

Research Group
Wenfeng Zhao, Graduate Student Researcher

Jie Hu, Principal Investigator

Implementation of Several Self-Organizing Map Algorithms

The self-organizing map (SOM) algorithm is widely used in many applications. However, computation on the SOM algorithm is time-consuming. For this reason, these researchers are investigating parallel implementation of this algorithm. They are using the SGI Origin 2000 to run several SOM algorithms that have proved to be convergent in theory.

Research Group
Qiang Zhang, Graduate Student Researcher

University of St. Thomas

Department of Engineering

John Abraham, Principal Investigator
Ephraim M. Sparrow, Co-Principal Investigator

A Numerical Investigation of Fluid Flow in Internally Baffled Channels

The use of internally baffled channels with high aspect ratios can provide very effective heat transfer coefficients. They are also characterized by high pressure gradients that currently limit their use. The goal of this project is to determine how to optimize pressure drop and heat transfer for such channel geometry in the application of cold-plate technology. The researchers are using the programs FLUENT and ANSYS on the supercomputers for their computations.

Research Group

Paul Chevalier, Graduate Student Researcher
Sandra Sparr, Graduate Student Researcher

Index and Bibliography

Index of Principal Investigators

Index of Principal Investigators

Index of Principal Investigators

Index of Principal Investigators

Bibliography

UMSI Research Reports, January 1, 2001–March 15, 2003
(arranged alphabetically by field of study)

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