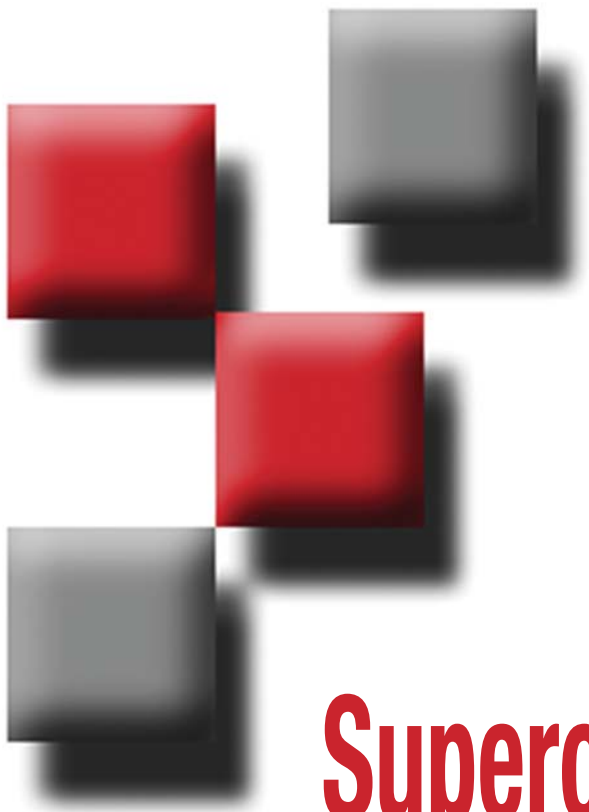


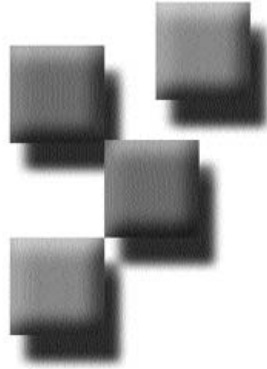


Supercomputing Institute

for Digital Simulation and Advanced Computation

2002 Annual Research Report

UNIVERSITY OF MINNESOTA



**2002 Annual Research Report of the
Supercomputing Institute
for Digital Simulation
and Advanced Computation**

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UNIVERSITY OF MINNESOTA

Supercomputing Institute
for Digital Simulation and Advanced Computation
University of Minnesota
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This report was prepared by Supercomputing Institute researchers and staff.
Editor: Tracey Bartlett

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Table of Contents

Introduction

Supercomputing Resources

Overview.....	2
Supercomputers	3
Research Laboratories and Programs	5

Supercomputing Institute Programs

Graduate Programs	10
Partnership	11
Digital Technology Center	12
Research Scholars.....	13
Undergraduate Interns.....	14

Researchers and Administration

Fellows of the Institute	16
National Advisory Board	18
Administrative Staff	19
Technical Support Staff	20
Committee and Panel Members	21
External Support	23

Conferences

Sponsored Symposia	30
--------------------------	----

Table of contents continued on next page.

Table of Contents

Ongoing and Recently Completed Research Projects from January 1, 2001 to March 15, 2002

University of Minnesota–Duluth Campus

College of Science and Engineering

Department of Chemistry	35
Department of Electrical and Computer Engineering	36
Department of Physics	37

University of Minnesota–Twin Cities Campus

College of Agricultural, Food, and Environmental Sciences

Department of Soil, Water, and Climate	39
--	----

College of Biological Sciences

Biotechnology Institute	42
-------------------------------	----

College of Biological Sciences and Medical School

Department of Biochemistry, Molecular Biology, and Biophysics	44
---	----

College of Liberal Arts

Department of Economics	61
Department of Geography	65
Department of Political Science	66

College of Natural Resources

Department of Wood and Paper Science	68
--	----

College of Pharmacy

College of Pharmacy	70
Department of Medicinal Chemistry	71
Department of Pharmaceutics	76

Curtis L. Carlson School of Management

Department of Finance	78
Department of Operations and Management Science	79

School of Public Health

Division of Epidemiology	81
--------------------------------	----

Institute of Technology

Department of Aerospace Engineering and Mechanics	86
Department of Astronomy	94
Department of Biomedical Engineering	97
Department of Chemical Engineering and Materials Science	99
Department of Chemistry and Chemical Physics Program	119
Department of Civil Engineering	139
St. Anthony Falls Laboratory	151
Department of Computer Science and Engineering	160
Department of Electrical and Computer Engineering	165
Department of Geology and Geophysics	173
Institute for Mathematics and Its Applications	177
School of Mathematics	178
Department of Mechanical Engineering	183
Department of Physics	202

Medical School

Cancer Center	217
Department of Laboratory Medicine and Pathology	218
Department of Neuroscience	224
Department of Orthopaedic Surgery	228
Department of Otolaryngology	229
Department of Pharmacology	230
Department of Physiology	232
Department of Radiology	235
Department of Surgery	237
Department of Therapeutic Radiology–Radiation Oncology	241

Mayo Medical School

Department of Pharmacology	243
----------------------------------	-----

Metropolitan State University

Department of Information and Computer Sciences	245
---	-----

Minnesota State University–Mankato

Department of Management	247
--------------------------------	-----

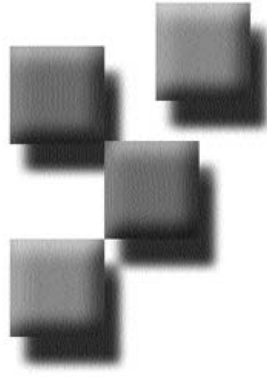
Index and Bibliography

Index of Principal Investigators

Index of Principal Investigators	250
--	-----

Research Reports Bibliography for January 1, 2001–March 15, 2002

Aerospace Engineering and Mechanics	252
Astronomy	253
Biochemistry, Molecular Biology, and Biophysics	254
Biomedical Engineering	255
Chemical Engineering and Materials Science	255
Chemistry	258
Civil Engineering	266
Computer Science and Engineering	268
Economics	270
Electrical and Computer Engineering	270
Epidemiology	272
Geology and Geophysics	272
Industrial Relations	275
Information and Computer Science	275
Laboratory Medicine and Pathology	276
Mathematics	277
Mechanical Engineering	278
Medicinal Chemistry	279
Microbiology	280
Operations and Management Science	280
Orthopaedic Surgery	280
Otolaryngology	281
Physics	281
Physiology	283
Political Science	283
Soil, Water, and Climate	284
Surgery	284
Wood and Paper Science	284



Introduction

Supercomputing Resources

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.

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 April 2000, the WinterHawk nodes were upgraded to WinterHawk+ technology. The Institute's IBM SP supercomputer currently comprises 390 processors with 663 GB of memory. It consists of 79 four-processor and 3 two-processor WinterHawk+ nodes with 391 GB of memory and 17 four-processor NightHawk nodes with 272 GB of memory. The NightHawk nodes utilize the 222 MHz Power3 processors and WinterHawk+ nodes utilize the 375 MHz Power3+ processor. 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. The IBM supercomputer resources are available in coordination with the IBM Shared University Research (SUR) partnership.

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.

In March 2002, the Supercomputing Institute purchased an IBM pSeries 690 (Regatta). This computer contains eight 1.3 GHz processors and has 16 GB of memory. In August 2002, this system will be upgraded to two Regattas. One will have 32 processors with 64 GB of memory, the other will have 24 processors and 24 GB of memory. These machines will be connected together using the SP Switch2.

The total amount of disk available to users of the IBM SP systems is 4.5 terabytes. The total amount of disk available to users of the SGI Origin 2000 systems is currently 3.0 terabytes.

The Institute recently added a Linux Cluster consisting of 82 2-processor Netfinity nodes from IBM. Of these 82 nodes, 76 are available for computation, 5 are file servers, and one node is for interactive use. 17 of these nodes have two 733 MHz 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.

The Supercomputing Institute recently joined the Digital Technology Center, and the supercomputing resources have moved to the Supercomputing Institute's new facilities on the East Bank of the Minneapolis Campus.

Supercomputers

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

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

Planning Committee

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

Graham Candler, Aerospace Engineering and Mechanics and Scientific Computation

James Chelikowsky, Chemical Engineering and Materials Science and Scientific Computation

Jiali Gao, Chemistry and Scientific Computation

Vipin Kumar, Computer Science and Engineering and Scientific Computation

David Lilja, Electrical and Computer Engineering

Alon V. McCormick, Chemical Engineering and Materials Science

Douglas Ohlendorf, Biochemistry, Molecular Biology, and Biophysics

Yousef Saad, Computer Science and Engineering and Scientific Computation

George Wilcox, Neuroscience and Scientific Computation

Research Laboratories and Programs

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 facility occupies approximately 1700 square feet that includes a workstation room, video/graphics room, machine room, and two offices. The laboratory houses state-of-the-art computing platforms and graphics workstations including 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 2001–02 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 Mayo, Biochemistry, Molecular Biology, and Biophysics, chair

Jiali Gao, Chemistry and Scientific Computation

David Live, Biochemistry, Molecular Biology, and Biophysics

Darrin York, Chemistry

George L. Wilcox, Neuroscience and Scientific Computation

Carrie Wilmot, Biochemistry, Molecular Biology and Biophysics

Research Laboratories and Programs

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 will be in St. Paul, and will be located in the new Microbial and Plant Genomics building when it is finished. There will also be a secondary home in the Basic Sciences and Biomedical Engineering Building. 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. A search for dedicated laboratory personnel is on-going, and laboratory activities will increase when a permanent manager is in place.

This laboratory was overseen and guided during 2001–2002 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 Berman, Genetics, Cell Biology, and Development

George Karypis, Computer Science and Engineering

Yiannis Kaznessis, Chemical Engineering and Materials Science

Arkady Khodursky, Biochemistry, Molecular Biology, and Biophysics

Lawrence Wackett, Biochemistry, Molecular Biology, and Biophysics

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 will allow 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 2001–2002 by the following committees:

Executive Committee

Hans Othmer, Mathematics and Scientific Computation, chair

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

Steering Committee

Hans Othmer, Mathematics and Scientific Computation, chair

Jiali Gao, Chemistry and Scientific Computation

Alexander Grosberg, Physics and Astronomy

John Lowengrub, Mathematics

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, an SGI O2 workstation for the creation and manipulation of videos, and a Super-VHS VCR. The Institute provides user support services for supercomputer-related research using these general-purpose systems.

For 2001–02, the Scientific Development and Visualization Laboratory was guided by a faculty steering committee made up of:

Thomas W. Jones, Astronomy and Scientific Computation, chair

Jiali Gao, Chemistry and Scientific Computation

Satish Gupta, Soil, Water, and Climate

Dan Kroll, Pharmacy

Gary Meyer, Computer Science and Engineering

Fernando Porté-Agel, Civil Engineering

Henryk K. Stolarski, Civil Engineering

Research Laboratories and Programs

IBM Shared University Research Netfinity Cluster

The initial period of deployment of the IBM Netfinity Cluster was guided by a special steering committee. In particular, for 2000–01 the IBM Shared University Research Netfinity Cluster Laboratory was guided by a faculty steering committee made up of:

Thomas W. Jones, Astronomy and Scientific Computation, chair

David Lilja, Electrical and Computer Engineering

J. Ilja Siepmann, Chemistry and Scientific Computation

Darrin M. York, Chemistry

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 scientific visualization. This laboratory was overseen and guided during 2001–02 by the following committees:

Executive Committee

Yusuf 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

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 technical support in the area computational biology, specifically including tutorials and seminars

IBM has awarded the Supercomputing Institute a Shared University Research (SUR) grant, which allowed the Institute to purchase a 7-terabyte disk.

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 first three affiliates are Cargill, the Hormel Institute, and the Mayo Medical School.

Further information about this program is available at:
<http://www.msi.edu/general/programs/uofmibm/index.html>

Supercomputing Institute Programs

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 Director of Graduate Studies in 2001–2002 was David Ferguson, Medicinal Chemistry.

Computational Neuroscience Training 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 Science Program is funded in part by a National Science Foundation Integrative Graduate Education and Research Training (IGERT) grant. The Executive Committee consists of Timothy J. Ebner, Neuroscience, and Donald G. Truhlar, Supercomputing Institute Director, Chemistry, Chemical Physics, and Scientific Computation.

Partnership

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 2001–02 by the following committees:

Executive Committee

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

Paul Woodward, Astronomy and Scientific Computation

Program Committee

Paul Woodward, Astronomy and Scientific Computation, chair

George Wilcox, Neuroscience and Scientific Computation

David Yuen, Geology and Geophysics and Scientific Computation

Digital Technology Center

The Supercomputing Institute is also playing a central role in the University of Minnesota's digital technology initiative. This initiative includes technologies based on computers, electronics, 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.

Supercomputing Institute Research Scholars

In addition to providing state-of-the-art supercomputing resources to the University of Minnesota research community, the Supercomputing Institute offers a Research Scholarship Program 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 eleven 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.

Over the past two years (2000–2001), the Supercomputing Institute awarded research scholarships to:

Titus V. Albu, Department of Chemistry

Pavel Belík, School of Mathematics

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

Fabien Dubuffet, Department of Geology and Geophysics

Witold Dzwiniel, Institute of Computer Science, A.G.H., Krakow, Poland

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

Anguang Hu, Department of Chemistry

Bijaya Karki, Department of Chemical Engineering and Materials Science

Leeor Kronik, Department of Chemical Engineering and Materials Science

Xabier Lopez, University of the Basque Country, Spain

Omid Mohseni, Department of Civil Engineering, St. Anthony Falls Laboratory

Hisao Nakamura, Department of Chemistry

Ilaria Perugia, Dipartimento di Matematica, Università di Pavia, Pavia, Italy

Jeffrey Potoff, Department of Chemistry

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 2001–02

Graham Candler, Aerospace Engineering and Mechanics and Scientific Computation, chair

Leonard Banaszak, Biochemistry, Molecular Biology, and Biophysics

John Lowengrub, Mathematics

J. Ilja Siepmann, Chemistry and Scientific Computation

Vaughan R. Voller, Civil Engineering

Pen-Chung Yew, Computer Science and Engineering

Supercomputing Institute Undergraduate Interns

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. This includes digital simulation and advanced computation; it 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. 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 414 interns in its thirteen years of existence.

Over the past two years (2000–01), the Supercomputing Institute awarded internships to the following undergraduates:

Anthony Anderson, University of Minnesota
Abdul Bahar, University of Minnesota
Victoria Bedell, Bethel College
Sarah Betterman, University of Minnesota
Nenad Bjeloglic, University of Minnesota
Adam Butensky-Bartlett, Northwestern University
Mira Chaurushiya, Carleton College
Claire Chisolm, University of Alabama-Tuscaloosa
Aron Cooper, University of Minnesota
Jedediah Deitrick, Kansas State University
Zachary Garbow, University of Minnesota
Michael Garrels, Case Western Reserve University
Pedro Gautier, Universidad Metropolitana, Bayamon, Paraguay
Loren Gragert, University of St. Thomas
Jerome Hauser, Princeton University
Peter Holm, Iowa State University
Eric Johnson, University of Minnesota
Nicholas Koshnick, Dartmouth College

Benjamin Langmead, Columbia University
Andrea Lay, Tulane University
Corey Maley, University of Nebraska–Lincoln
Daniel Melendez, Universidad Metropolitana, Bayamon, Paraguay
John O’Leary, University of Chicago
Mariah Olson, University of Minnesota
Nick Olson, University of Maryland
Peter Oman, University of Minnesota
Jonathan Othmer, Williams College
David Joseph Regelman, Stanford University
William Ryan, Rice University
Matthew Salomane, Northwestern University
Dawn Schafer, Bethel College
Nathan Schultz, St. John’s University and the College of St. Benedict
Sundee Shaky, University of Mississippi
Timothy Sonbuchner, Gustavus Adolphus College
Samuel Stechmann, University of Saint Thomas
Andrew Watson, University of Minnesota

Undergraduate Internship Program Committee for 2001–02

William Gleason, Laboratory Medicine and Pathology, chair
David Thomas, Biochemistry, Molecular Biology, and Biophysics and Scientific Computation
Donald G. Truhlar, Supercomputing Institute Director,
Chemistry, Chemical Physics, and Scientific Computation

Researchers and Administration

Fellows of the Institute

Fellows

Douglas Arnold
Daniel L. Boley
Graham Candler
James R. Chelikowsky
Bernardo Cockburn
Christopher Cramer
H. Ted Davis
Jeffrey Derby
David Du
David Ferguson
Efi Foufoula-Georgiou
Jiali Gao
William Gleason
Alexander Grosberg
J. Woods Halley
Dennis Hejhal
Thomas W. Jones
Daniel D. Joseph
Thomas H. Kuehn
Vipin Kumar

David J. Lilja
John S. Lowengrub
Mitchell B. Luskin
Alon McCormick
Douglas Ohlendorf
Hans Othmer
Suhas Patankar
J. Ben Rosen
Yousef Saad
L. E. Scriven
George Sell
J. Ilja Siepmann
Charles C. S. Song
Kumar K. Tamma
David D. Thomas
Donald G. Truhlar
Oriol T. Valls
Renata Wentzcovitch
George Wilcox
Paul Woodward
David A. Yuen

Adjunct Fellow

Philippe de Forcrand

Associate Fellows

Larry D. Atwood

Leonard J. Banaszak

Charles E. Campbell

Robert W. Carr

Cynthia A. Cattell

Roger Fosdick

William W. Gerberich

Steven L. Girshick

Richard Goldstein

Anand Gopinath

Gautam Gowrisankaran

Satish C. Gupta

Bojan Guzina

Jerome Hajjar

Franz Halberg

Joachim V. Heberlein

John R. Hiller

Wei-Shou Hu

Peter J. Hudleston

Steven R. Kass

Paul Kiprof

Katherine Klink

Uwe Kortshagen

Joseph F. Labuz

James R. Leger

Perry H. Leo

David Levitt

Robert L. Lysak

Christopher W. Macosko

Brian P. McCall

Peter H. McMurry

John Nieber

David Y.H. Pui

P. Paul Ruden

Lanny D. Schmidt

Terrence W. Simon

Friedrich Srien

Heinz G. Stefan

Henryk K. Stolarski

Robert Tranquillo

Vaughan R. Voller

Yiyuan Zhao

National Advisory Board

The National Advisory Board, made up of national experts in several areas of high-performance computing, had three members in 2001:

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

DTC Administrative Director for Human Resources

Ann Johns

Executive Secretary

Barbara Van Eps

Accountant

Brian Carlton

Editor and Undergraduate Internship Program Coordinator

Tracey Bartlett

Executive Administrative Specialist

Annice Larkin

Secretarial Assistant

Jessica Dziewecynski

DTC/MSI Principal Administrative Specialist/Receptionist

Marni Anderson

Technical Support Staff

Manager of Operations and User Support

Barry Schaudt

Scientific Computation User Support Specialists

Patton Fast

Cal Kirchhof

Birali Runesha

Marina Sapir

Yuk Sham

Zheng Jin Tu

Shuxia Zhang

Operations Staff

Dack Anderson

John Boggs

Kirk Deen

Richard Flesvig

Yectli Huerta

Thomas Kniffen

Stefan Parnell

Samantha Thomas

Gabe Turner

Committee and Panel Members 2000-2002

Yusuf Abul-Hajj, Medicinal Chemistry
Leonard Banaszak, Biochemistry, Molecular Biology, and Biophysics
Judith Berman, Genetics, Cell Biology, and Development
Daniel L. Boley, Computer Science and Engineering and Scientific Computation
Graham Candler, Aerospace Engineering and Mechanics and Scientific Computation
Cynthia A. Cattell, Physics
James Chelikowsky, Chemical Engineering and Materials Science and Scientific Computation
Bernardo Cockburn, Mathematics and Scientific Computation
Prodromos Daoutidis, Chemical Engineering and Materials Science
Jeffrey J. Derby, Chemical Engineering and Materials Science and Scientific Computation
Jiali Gao, Chemistry and Scientific Computation
Sean C. Garrick, Mechanical Engineering
William Gleason, Laboratory Medicine and Pathology
David J. W. Grant, Pharmaceutics
Alexander Grosberg, Physics and Astronomy
Satish 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 Engineerings
Steven R. Kass, Chemistry
Yiannis Kaznessis, Chemical Engineering and Materials Science
Katherine Klink, Geography
Arkady Khodursky, Biochemistry, Molecular Biology, and Biophysics
Dan Kroll, Pharmacy
Vipin Kumar, Computer Science and Engineering and Scientific Computation
David Lilja, Electrical and Computer Engineering

Committee and Panel Members 2000–2002

David Live, Biochemistry, Molecular Biology, and Biophysics

John Lowengrub, Mathematics

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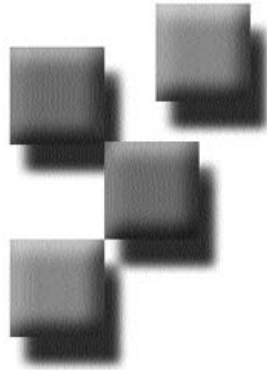
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Ongoing and Recently Completed Research Projects

January 1, 2001 to March 15, 2002

University of Minnesota—Duluth

College of Science and Engineering

Department of Chemistry

Paul Kiprof 35

Department of Electrical and Computer Engineering

Masha Sosonkina 36

Department of Physics

John R. Hiller 37

Paul Kiprof, Associate Fellow

Silene Cycloaddition Reactions

This research group studied the reaction of silicon-carbon double bonds with other molecules that have multiple bonds at high levels of theory by using *ab initio* molecular orbital programs such as GAMESS and GAUSSIAN. The group's emphasis is on the reactions of silene with acetylene and ethylene. These reactions were discovered recently and pose 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 can be carried out thermally in the dark. The concerted transition state for reactions have been studied. These researchers were also concerned with the alternative step-wise pathways of the reaction, which involve stable intermediates.

These researchers are also investigating high-valent transition metal arene complexes and carbocations. High-valent transition metal arene complexes are rare and generally unstable compared with their low-valent counterparts. A detailed study of the factors governing the stability of these complexes is being performed at high levels of theory accounting for the effect of substituents.

Further research involves carbocations, which are stabilized by oxygen atoms. This stabilization leads to unusual reactions that have not been studied systematically. This research group will explore the effect of the heteroatoms at high levels of theory and study the reactions that these species undergo. ■

Research Group

Sergiy Krasutsky, Undergraduate Student Researcher
Stephan Miller, Graduate Student Researcher
Kyle Riess, Undergraduate Student Researcher

Masha Sosonkina, Principal Investigator

Providing Dynamic Network Information to Distributed Applications

Clusters of personal computers provide an inexpensive alternative to high performance computing. However, the sustained performance of these computational and network resources is difficult to ensure for the total execution time of an application. Due to numerous factors, sudden changes in the amount of available resources are common, and this situation affects the running application.

To cope with fluctuations in hardware performance, an application may need to have adaptive capabilities. This is especially vital for scientific applications, since the majority of them are characterized by long execution times and by expensive recoveries from failure.

These researchers investigated the interaction between running scientific applications and the network interconnecting distributed computing resources. In particular, these researchers applied iterative methods to solve linear systems arising in static tire equilibrium computation. The heterogeneous material properties, nonlinear constraints, and a three-dimensional finite element formulation made the linear systems arising in tire design difficult to solve by iterative methods. An analysis of the matrix characteristics helped understand this behavior. Focusing on two preconditioning techniques, a variation of an incomplete factorization with threshold and a multilevel recursive solver, the researchers adapted these techniques in a number of ways to work for a class of realistic applications.

It was found that these preconditioners improve convergence only when a rather large shift value is added to the matrix diagonal. A combination of other techniques—such as filtering of small entries, pivoting in preconditioning, and a special way of defining levels for the multilevel recursive solver—were shown to make these preconditioning strategies efficient for problems in tire design. Comparisons were made between these techniques, and their

applicability was assessed in circumstances where the linear system difficulty varied for the same class of problems.

In related research, this group investigated means to improve the performance of distributed-memory architectures used by scientific applications. Distributed computations are widely used to solve large-scale realistic problems in scientific applications. By using standard communication libraries, such as Message Passing Interface (MPI), distributed scientific applications are made portable across various network and shared-memory interconnections of processors. For distributed-memory architectures, the performance of applications may vary greatly due to the different performances of various network technologies. Not only static (configuration) network characteristics, but also dynamically changing conditions such as network load, may affect the performance. For an application, one way to react to the dynamic network changes is to adjust its own communication needs. However, distributed (scientific) applications typically have no embedded means to learn the current network conditions. Therefore, it is desirable to have a mechanism that provides the network information transparently to the application programmer or user, so that the burden of handling the low-level network information is shifted to a network developer. ■

Research Group

Devdatta Kilkarni, Graduate Student Researcher

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Nonperturbative Analysis of Field Theories Quantized on the Light Cone

Quantum field theories 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 spacial 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. In this project two different methods for the removal of such infinities are being explored. 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 to not 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.

Progress in the application of Pauli-Villars regularization included the nonperturbative solution of (3+1)-dimensional Yukawa theory in a single-fermion truncation. Three heavy scalars, including two with negative norm, were used to regulate the theory. The numerical eigenvalue problem was solved for the lowest-mass state with use of a new, indefinite-metric Lanczos algorithm. Various observables were extracted from the wave functions, including average multiplicities and average momenta of constituents, structure functions, and a form factor slope. The most recent work introduces an improved regularization scheme that uses one heavy scalar and one heavy fermion. This method has been shown to have the distinct advantage of eliminating the instantaneous fermion terms from the Hamiltonian. These

terms cancel between the physical and Pauli-Villars fermions but would otherwise contribute the bulk of the nonzero Hamiltonian matrix elements. Preliminary results show much better convergence than seen with the original regularization. The better convergence is at least partly due to the absence of the instantaneous-fermion interactions.

In the work on supersymmetric theories, this researcher completed an in-depth study of the spectrum and wave functions for (2+1)-dimensional supersymmetric Yang-Mills theory. He has begun a new analysis for the theory obtained by adding a Chern-Simons term. This term provides the constituents with an effective mass without breaking the supersymmetry. The resulting theory has a spectrum that is more comparable to strong interaction physics, where the fundamental quarks and gluons do have effective masses. The researcher has also completed a study of a dimensionally reduced version of the super Yang-Mills-Chern-Simons theory, with the discovery of states in the spectrum for which the masses are nearly independent of the Yang-Mills coupling strength. Such states are expected to be found in the ongoing analysis of the full (2+1)-dimensional spectrum. ■

University of Minnesota—Twin Cities

College of Agriculture, Food and Environmental Sciences

Department of Soil, Water, and Climate

Satish C. Gupta.....39

Dong Wang 40

Satish C. Gupta, Associate Fellow

Quantifying Riverbank Erosion Using Airborne Scanning Laser Altimetry

The Minnesota River flows through a 95% agricultural watershed, yet it has been ranked among the 20 most polluted rivers in the U.S. The river flows through a relatively flat 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-à-vis stream bank collapse. This study is designed to determine the feasibility of using a helicopter-mounted scanning laser to estimate riverbank erosion. Specifically, this research group is measuring bank erosion along the Blue Earth River in southern Minnesota; this river contributes 55% of the sediment load to the Minnesota River at Mankato. The procedure involves two laser scans, taken one year apart, of the Blue Earth River valley. The difference in the elevations between scans quantifies the extent of banks that may have eroded or sloughed during that time period.

In April 2001, the research group made the first scan of a 35-mile length of the Blue Earth River from Amboy to Rapidan Dam. They have constructed the digital elevation model of the river and have also made an animation of the river valley. The figure shows an example of the raw elevation data for two riverbanks along the Blue Earth River. The group will make a second scan of the riverbanks in Spring 2002. They will use the difference in elevations between the two scans to estimate bank erosion during the last year. They have also made bulk density measurements on the riverbanks and will be using these to convert volume change into sediment loads. ■



Laser scan of two riverbanks on the Blue Earth River.

Research Group and Collaborator

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

The dynamics of pesticide volatilization is strongly controlled by subsurface transport and ambient environmental conditions, which may be described with process-based 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. However, 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. These researchers are integrating an existing comprehensive two-dimensional pesticide simulation model with management selections by adopting the most efficient numerical schemes. ■

Research Group

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Biotechnology Institute

Friedrich Sienec	42
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Friedrich Srienc, Associate Fellow

Cell Growth Dynamics of Unicellular Organisms Under Changing Environmental Conditions and Elementary Mode Analysis for Biochemical Networks

Cell properties such as mass, protein content, 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 next step was to extend 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. 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 ($\partial c/\partial t=0$) on internal metabolites,

where c is concentration and t is time. 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 significant computational burden, making the use of Supercomputing Institute resources necessary. ■

Research Group and Collaborator

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Ian M. Armitage	44
Leonard J. Banaszak	45
Bridgette A. Barry.....	47
Victor Bloomfield	48
Bianca M. Conti-Fine.....	49
Alex J. Lange.....	50
John D. Lipscomb	51
David Live.....	52
Kevin Mayo.....	53
Douglas H. Ohlendorf	54
Osha Roopnarine	56
David D. Thomas.....	57
Kylie J. Walters.....	58
Carrie Wilmot	59

Ian M. Armitage, Principal Investigator

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

This research group is using biomolecular nuclear magnetic resonance (NMR) methods to investigate: the structure and metal exchange properties of proteins involved in the maintenance of metal homeostasis *in vivo*; the structure and function of select molecules involved in the immune response; and the structure, dynamics, and mechanism of activation of specific zinc finger deoxyribonucleic acid (DNA) transcription factors upon zinc binding.

The team used computational resources of the Basic Sciences Computing Laboratory (BSCL) to process of multidimensional NMR data sets, calculate the three-dimensional biomolecular structure, and visualize calculated structure. ■

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Structure and Function Studies of Biological Macromolecules

The link between the biological function and the conformation of protein molecules is still not well established. To make the connection and to understand the chemical properties of proteins, this research team studied the conformation of selected protein molecules by macromolecular x-ray crystallography. Such direct conformational determinations by x-ray diffraction methods are computationally intensive and require the use of supercomputer resources. However, the results proved startling in that thousands of connected atoms may be positioned according to their orientation in living organisms. Since each protein molecule has a specific task, studies continued to develop information on the structure:task relationship. Because a human being has somewhere between 30,000 and 40,000 different proteins, structural biology is divided into different areas related to the tasks of the various proteins.

This team of scientists was made up of graduate and undergraduate students, post-doctoral fellows and staff scientists. A variety of studies were undertaken, each focusing on a structure:task problem in biology. In terms of their overall focus, three areas stand out:

- Using the structural biology tools, lipid transport and metabolism were studied. Toward this goal, the researchers' efforts focused on understanding the atomic basis for fat transport and breakdown. Not only were molecular structures determined, but attempts are now also being made to redesign proteins that bind lipids, as well as to explain the result of certain genetic disorders.
- Many proteins are also classified as enzymes or living chemical catalysts. Once the molecular structure is determined, further studies may reveal the atomic mechanisms by which the chemical reactions are catalyzed and the molecular changes that are necessary to control the catalytic reaction.
- In cells found in higher organisms, both in plants and animals, some proteins are synthesized and then must be "directed and translocated" to an appropriate organelle. An organelle is a subparticle within a cell generally responsible for some overall physiological function. For example, chloroplasts in plants contain the proteins responsible for photosynthesis. In animals and plants, mitochondria are organelles responsible for energy production. Each contains a different array of proteins. Using x-ray crystallography, studies were made to determine how different proteins are sorted to their appropriate organelle within the cell.

In the first group, studies focused on adipocyte lipid binding protein (ALBP), cellular retinoic acid binding protein (CRABPI), lipovitellin (LV), and microsomal triglyceride transfer protein complexed with protein disulfide isomerase (MTP:PDI). To illustrate the magnitude of the determination and visualization problem, lipovitellin is a molecule that contains 1,500 amino acids of which there are 20 different kinds. The "average" amino acid contains seven atoms, excluding hydrogens. Hence, to determine the molecular structure, the positions of about 10,500 heavy atoms must be located.

Also in this area, the researchers partially accounted for species variation and the accommodation of different ligands in the family of proteins known as the fatty acid binding proteins (ALBP, CRABPI, etc.) in the crystal structure of rat liver fatty acid binding protein (LFABP). An alignment of amino acid sequences of all known species was used to demonstrate two groups of sub-classes. Based on estimates at neutral pH and the electrostatic field calculated using the crystal coordinates,

Leonard J. Banaszak, Associate Fellow

some evidence of changes that occur in going from holo- to apo-forms was obtained. LFABP, unlike other family members, has two fatty acid binding sites. The two cavity sites were reviewed and arguments for interactions between the sites were developed. Finally, hypothetical models were built of complexes of LFABP and heme, and LFABP and oleoyl CoA. In both cases, the stoichiometry was one to one and the models exhibited why this is likely.

By changing specific atoms in the overall structure, attempts have been made to understand how two protein homologues may have different binding affinity. For example, one family member may bind fatty acids (ALBP) while another prefers retinoic acid (CRABPI). By careful studies of the molecular structures, attempts have been made to change the properties of one protein into another.

In the second area, projects on the enzymes malate dehydrogenase (MDH), short chain L-3-hydroxyacyl CoA dehydrogenase (SCHAD), phosphoglycerate dehydrogenase (PGDH), isocitrate dehydrogenase (IDH), and isocitrate dehydrogenase kinase/phosphatase (IDHKP) were undertaken. With the goal of understanding the molecular basis for catalytic activity and catabolite control, a number of crystal structures have been determined and refined, taking advantage of the Basic Sciences Computing Laboratory (BSCL) resource of the Supercomputing Institute. The SCHAD project offers a good example of how a structural study proceeds. After the initial three-dimensional structure was determined, further studies focused on determining the binding sites for the compounds that are catalytically changed by the protein. A series of x-ray studies showed that a small rearrangement of the conformation took place during a catalytic cycle. It also described the molecular basis for human disorders that result from single site mutations in the enzyme.

Enzymes may be regulated in different ways. For example, the enzyme IDH is inhibited by phosphorylation. The organism senses the need to turn off the catalyst (IDH) and another protein modifies IDH by adding four additional atoms. Hence a catalyst containing thousands of atoms is temporarily inhibited by a relatively simple chemical modification. Computational resources of the Supercomputing Institute/BSCL were used extensively in the comparison of the IDH to different organisms. Another enzyme, PGDH, is controlled by binding the end product of the pathway. Studies describing three-dimensional changes that accompany the binding process were nearing completion. Eventually these results will explain a major issue in the control of biological catalysts.

In the third category, structural studies focused on the comparison of molecules that may be translocated with those that are not. Again, these protein molecules contain thousands of atoms and the resources of the Supercomputing Institute are in constant demand. ■

Research Group and Collaborators

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Bridgette A. Barry, 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 electron transfer reactions in photosynthetic reaction centers. This research group is performing density functional calculations to determine the electronic structure of neutral tyrosyl radicals and chlorophyll cation radicals. Calculations will be performed in the gas phase and in the presence and absence of key hydrogen-bonding interactions. From the calculations, spectroscopic properties of experimental interest, such as vibrational frequencies, isotope shifts, and hyperfine coupling constants, will be derived. Comparison with experimental data, acquired from photosynthetic reaction centers and from model compounds in solution, will give insight into the structure and function of these species in photosynthetic reaction centers. These calculations will set the stage for future work exploring the nature of electron transfer intermediates using a hybrid quantum mechanical/molecular mechanical approach. ■

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Victor Bloomfield, Principal Investigator

Preferential Solvation: A Method for Obtaining Cosolvent and Water Concentrations at a Macromolecular Surface

Mixed solvent systems are important in the understanding of the structures and stabilities of macromolecules. For example, urea and guanidine HCl have long been used to study protein denaturation; alcohols are condensing agents for deoxyribonucleic acid (DNA). To understand cosolvent-macromolecular interactions, it is necessary to determine where cosolvents are—do they tend to lie within the bulk solvent or do they prefer to associate with the macromolecule? The preferential solvation (PS) measurement is a potential method for obtaining the water/cosolvent composition near a macromolecular surface. PS measures the amount of cosolvent and water in the environs of the macromolecule.

PS data are available for many cosolvents with many proteins; the Bloomfield lab gathered further data on cosolvents with DNA. Unfortunately, interpreting PS data is not straightforward. Current theories are limited in their practicality and have yet to be tested against known solvent distributions. Despite the wealth of PS data, no one had yet used these data to determine where cosolvents lie. The goals of this project were to develop a practical method for obtaining the cosolvent/water composition at a macromolecular surface from PS measurements and to test existing theories. Simulations are ideal for this purpose because it is difficult to obtain the solvent distributions from purely experimental methods.

The first step toward understanding PS was to determine the excluded-volume contribution. When cosolvents and waters have different sizes, it is well known that the surface cosolvent:water distribution is not like that of the bulk solvent. What portion of preferential solvation is due to size differences alone as opposed to interactions? To answer this ques-

tion, these researchers followed their earlier work by running grand-canonical Monte Carlo simulations (using cell lists) of binary mixtures of two-dimensional hard circular disks up against a hard wall. They then studied mixtures of three-dimensional hard spheres. The researchers tested existing preferential solvation theories by simulating many size ratios and compositions to mimic experimental systems. These simulations are CPU-intensive because of large size ratios and low concentrations of the large disks/spheres.

After determining the excluded-volume part of preferential solvation, the researchers added short-ranged interactions—van der Waals and hydrogen-bonding interactions—and, later, long-ranged interactions such as electrostatics to understand how each of these interactions contribute to PS. ■

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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 are able to cross-react with epitopes from self antigens.

In this laboratory, the researchers propagated from healthy subjects monoclonal CD4⁺ T cell lines that are able to recognize the same unrelated sequences. Each T cell clone expresses a different TCR, as judged by the sequence of its V α and V β regions. These researchers identified the sequence of the V α and V β regions of several such cross-reactive TCRs.

The goal of this project was to take advantage of the coordinates of the many solved TCR structures to model the sequences obtained, in an attempt to identify characteristics that would explain their cross-reactivity with unrelated sequences. ■

Research Group

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Description of Bisphosphatase Activity Modulations of the C-terminus in the Bifunctional Enzyme 6-Phosphofructo-2-kinase/fructose-2,6-bisphosphatase

The bifunctional enzyme, 6-phosphofructo-2-kinase/fructose-2,6-bisphosphatase, plays a crucial role in the regulation of glucose levels. It is the sole enzyme responsible for the synthesis and degradation of fructose-2,6-bisphosphate, a potent intracellular modulator of hepatic carbon flux. Fructose-2,6-bisphosphate is an allosteric activator of the glycolytic enzyme 6-phosphofructo-1-kinase and an inhibitor of the gluconeogenic enzyme fructose-1,6-bisphosphatase. The metabolic effects of glucagons, via cAMP-dependent protein kinase (where cAMP is cyclic adenosine monophosphate), on hepatic carbon flux are mediated by the intracellular concentration of fructose-1,6-bisphosphate. In diabetes, the excessive production of glucose by the liver is a major contributor to hyperglycemia, which leads to the major problems associated with the disease. The central role of fructose-2,6-bisphosphate in control of hepatic glucose levels will be beneficial to the diabetic patient. This group is investigating the efficacy of targeting the bisphosphatase domain of the bifunctional enzyme for inhibition, and thereby increasing the fructose-2,6-bisphosphate levels. The current model for an inhibited bisphosphatase has the phospho-accepting histidine mutated to alanine. Overexpression of this mutant in murine models of diabetes using an adenovirus vector has resulted in a normalization of blood glucose levels.

The Lange group is using Supercomputing Institute resources to process and display nuclear magnetic resonance data on the bisphosphatase domain of bifunctional enzyme, in order to characterize the active site and defining the catalytic mechanism(s). The group has identified the roles of the catalytic histidines and an active site glutamatic acid residue. Using ^{13}C and ^{15}N labeling of the histidine ring together with mutagenesis, the pro-

tonation and tautomeric states of the histidines and perturbations of the active site cause by mutating the glutamatic acid to alanine were determined.

The group's present work is pursuing the sequential assignment of the bisphosphate domain that will facilitate solving a solution structure and further biophysical characterizations. Concurrently, a spectroscopic investigation of the arginine residues in the active site utilizing specific labeling of the histidines and arginines is proceeding. Knowledge of this important component of gluconeogenic/glycolytic flux helps provides the basis for the rational design of specific inhibitors of the bisphosphatase activity of hepatic 6-phosphofructo-2-kinase/fructose-2,6-bisphosphate. ■

Research Group and Collaborator

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Structure and Mechanism of Oxygenase Enzymes

Oxygenase enzymes utilize molecular oxygen to oxidize a wide range of biological and man-made compounds with the incorporation of one or both atoms of oxygen from molecular oxygen in the products.

In the first project undertaken by this group, a series of dioxygenase enzymes was studied. These enzymes attack aromatic substrates with two hydroxyl substituents. The products are ring-open compounds containing both atoms of oxygen from O₂. Their 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 Ohlendorf's group, the researchers solved the crystal structures of three of these enzymes. Supercomputing Institute resources were used to examine the crystal structures and plan ongoing, site-directed mutagenesis studies.

The second class of oxygenase studied was typified by methane monooxygenase. This enzyme catalyzes the oxidation of methane to methanol with the incorporation of one atom of oxygen. Methane is generated in large quantities in the environment and is a potent greenhouse gas. It is prevented from reaching the atmosphere by the action of methane monooxygenase. Again in collaboration with Douglas Ohlendorf, the group solved the crystal structure of the critical hydroxylase component. Supercomputing Institute resources were used to visualize the structure and plan mutagenesis studies. ■

Research Group

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Structural Refinement of Glycoproteins

An important class of glycoproteins contains those with mucin-like domains, characterized by clusters of glycosylated serine and threonine residues. These are significant components on the cell surface. These researchers determined the structure of glycopeptide fragments by nuclear magnetic resonance methods in order to understand mucin glycoprotein organization. Supercomputing resources were used to aid in the structure refinement, using experimental constraints. ■

Collaborator

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Kevin Mayo, Principal Investigator

Structure and Dynamics of Proteins and Peptides

This group investigated the structure and dynamics of proteins and peptides by using nuclear magnetic resonance (NMR) spectroscopy. Following derivation of internuclear distance and angular constraints from various NMR experiments, computational modeling was performed in order to derive the best set of structures from the experimental data. Simulated annealing and molecular dynamics calculations were used in the protocol to derive the structure, and relaxation matrix calculations were used during structural refinement. In related work, this laboratory furthered the understanding of internal motions in proteins and peptides. In particular, molecular dynamics simulations were used in conjunction with NMR relaxation experiments on isotopically enriched peptides and proteins, in order to derive information on the motional frequencies and amplitudes of backbone and side-chain bond vectors. ■

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Douglas H. Ohlendorf, Fellow

Structural Biology 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 were checked through biophysical analysis of complexes and mutants of targeted proteins.

In recent work, the structural analysis of macromolecules was carried out in order to understand the structural basis of how macromolecules function. The current focus is on seven proteins—protocatechuate 3,4-dioxygenase (PCD), homoprotocatechuate 2,3-dioxygenase (HPCD), 1,2-catechol dioxygenase (CTD), toxic shock syndrome toxin-1 (TSST-1), streptococcal pyrogenic exotoxin A (SPEA), exfoliative toxin A (ETA), and exfoliative toxin B (ETB). The researchers used the computational resources of the Supercomputing Institute to refine structures of substrate and inhibitor complexes of PCD; to solve and refine the structures of HPCD, CTD, SPEA, ETA, ETB, and mutants to TSST-1, ETA, ETB, and PDC; and to model the structures of other dioxygenases and superantigens.

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 cleavage is adjacent to the vicinal hydroxyls (extradiol) and utilizes a non-heme Fe^{+2} ion or a Mn^{+2} ion. Work on this protein is focused on metal specificity as well as substrate selectivity.

Like PCD, CTD is an intradiol dioxygenase incorporating both atoms of molecular oxygen into an organic substrate using a non-heme ferric ion. However, where the PCDs being studied contain six or more protomers 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.

Toxic shock syndrome toxin-1 (TSST-1), from *Staphylococcus aureus*, is the causative agent in toxic shock syndrome and is a member of a family of pyrogenic toxins that have been referred to as superantigens. Typically 0.0001%–0.01% of helper CD4^{+} T-cells respond when presented with an antigen. However, when a superantigen such as TSST-1 is present, as many as 20% of these helper T-cells respond by releasing large amounts of cytokines producing fever, vomiting, diarrhea, shock, and sometimes death. Through the production of mutants of TSST-1, the researchers hope to be able to modulate these activities.

SPEA from *Streptococcus pyogenes* is the causative agent of toxic shock-like syndrome. This syndrome is 60–80% fatal and is the disease that killed the entertainer Jim Henson. Through analysis of the structure of SPEA in light of those of other superantigens (e.g., TSST-1), the researchers hope to discover the structural foundations for biological activities.

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. ■

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Correlation of EPR Spectroscopic Dynamics and Computer Simulated Molecular Dynamics of Mutations That Cause Heart Disease

Several different point mutations in the myosin heavy chain and light chains (LC) cause the human heart disease known as familial hypertrophic cardiomyopathy (FHC). The goal of this research was to understand the biophysical and biochemical basis of the mutant phenotypes by performing site-directed spin labeling (SDSL) and electron paramagnetic resonance (EPR) spectroscopy on FHC-mutant RLC in muscle fibers. The research is intended to determine the effect of the FHC mutations on the protein structure by simulating the mutations in crystal structures of myosin to ascertain whether or not the tertiary structure of the protein is affected by the mutation. Using the molecular modeling program INSIGHTII to construct energy-minimized models for the LC domain containing these rat VRLC mutations, this researcher planned to engineer cysteine residues on the crystal structures of the protein to determine if it is an appropriate site for minimal protein structural perturbation. This would allow development of an experimental design of spectroscopic studies. The simulated Cys mutants would then be used as the background for the FHC mutations. Following this work, the molecular dynamics program was expected to simulate the dynamics of a spin label attached to the Cys, in order to determine if the site for labeling would detect specific motional changes within the protein.

Preliminary work with the FHC-RLC mutations allowed the visualization of probable structures and the performance of molecular dynamics simulations to be compared directly with EPR spectroscopic data. The results of this were expected to suggest that the FHC mutation perturbs the flexibility of the region that connects the two principal lobes of the RLC. ■

David D. Thomas, Fellow

Computational Simulation of Muscle Protein Dynamics

Recent experiments using electron paramagnetic resonance (EPR) spectroscopy indicate a rotation of the myosin light chain domain during muscle contraction. EPR techniques measure the orientation of a spin label attached to the protein at any location. The researchers predicted optimal sites for labeling the myosin molecule by calculating an order parameter and simulating the EPR spectra based on the orientation of a spin label during molecular dynamics simulations.

Simulations can also provide the orientation of the spin label with respect to the actin protein axis, while experiments are limited to describing relative changes in the molecule's orientation. These computational techniques improve experimental efficiency and further the understanding of structural changes in molecules during muscle contraction.

As part of their study in muscle biomolecular dynamics, the research group set out to understand the molecular dynamics of force generation and movement in muscle. The group deduced the orientation and mobility of contractile proteins by examining and deconvoluting the EPR spectra and anisotropy decays of spin labels and optical probes attached to the particular components. Additionally, they tested models of molecular motion by simulating the EPR spectra and anisotropy decays predicted by the models. ■

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

This research group is using nuclear magnetic resonance (NMR) spectroscopy to reveal protein structures and protein-protein interactions. Projects in the lab focus on proteins associated with human cancers, with the aim of using structural knowledge to design molecular inhibitors against specific oncoproteins. One major topic of the lab 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 group is using their structural knowledge of the dimerization domain of a fusion protein associated with AML to design a molecular inhibitor that blocks dimerization.

Additionally, this group is 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 that 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 XPC (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. The group is solving the solution structure of the 40 kDa hHR23 protein. Furthermore, by using NMR spec-

troscopy, they are elucidating the proteasome-binding surface of hHR23. Using this knowledge, the group intends to design mutant versions of hHR23 that no longer bind the proteasome to be used in in vivo assays to ascertain the relevance of the hHR23-proteasome interaction in NER. ■

Research Group

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Carrie 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 cofactors and metal ions, as well as 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.

The research group intends to study structural enzymology involving the cofactor tryptophan tryptophylquinone (TTQ) of methyldiamine dehydrogenase (MADH), structural enzymology of the dinuclear copper-containing enzyme tyrosinase, and the role of copper redox chemistry in the progression of Alzheimer’s disease. ■

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Michele Boldrin	61
Varadarajan V. Chari.....	62
Varadarajan V. Chari and Michael P. Keane	63
Gautam Gowrisankaran	64

Department of Geography

Katherine Klink	65
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Department of Political Science

Diana Richards	66
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Michele Boldrin, Principal Investigator

The Cost of the Business Cycle

This research group investigated the cost of the business cycle in a heterogeneously educated household economy. The group 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 group used the facilities of the Supercomputing Institute to solve the associated Bellman equation, which contains a large number of state variables. ■

Collaborator

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Varadarajan V. Chari, Principal Investigator

Solving and Estimating Dynamic General Equilibrium Models with Heterogeneity

This research group applied Bayesian statistics tools that they had developed in their previous work at the Supercomputing Institute to estimate and compare a set of sticky price models widely used in the literature. Their results were presented in a paper entitled “How Important Are Real Wage Rigidities? A Bayesian Approach.”

The main results of the research were:

- The researchers’ model delivers reasonable point estimates for the duration of prices and wages, of three and five quarters respectively. The fraction of wage setters that follow a real wage indexing rule is about one half.
- As real wage rigidities are removed, the estimated duration of prices increases to high levels. The researchers view this result as a natural consequence to substitute for the lack of endogenous persistence associated with real wage rigidities.
- The group’s estimates point at little evidence suggesting backward-looking behavior in the inflation equation.
- Using the marginal likelihood of the data implied by each model, the model presented in this paper performs best.

A second project involved working on a method to perform nonlinear likelihood-based inferences in Dynamic Equilibrium Economies. Although this type of model is a standard tool in quantitative economics, existing literature has been forced so far to use moment procedures or linearization techniques to estimate these models. The researchers used Monte Carlo filtering to evaluate the likelihood function implied by the nonlinear solution of the model. As a consequence, they could perform likelihood-based inference, either searching for

a maximum (Quasi-Maximum Likelihood Estimation) or simulating the posterior using a Markov Chain Monte Carlo algorithm (Bayesian Estimation). ■

Research Group

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Varadarajan V. Chari, Principal Investigator Michael P. Keane, Co-Principal Investigator

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

This research concentrated on developing new methods to solve and estimate discrete stochastic dynamic programming (DS-SP) models and use these to study occupational and educational choices. 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-SP problem to determine their optimal decisions. However, empirical implementation of such models has been hampered because their solution and estimation requires that very high-order numerical integrations be performed.

This research investigated the use of simulation methods to circumvent these integration problems. These methods were employed in three substantive projects. The first was a model of life cycle decisions of young women; the focus was on their human capital investment (i.e., school attendance and work), fertility and marriage decisions, and how these are affected by public welfare programs. After this model was completed, it was found to be useful for predicting the effects of changes in welfare rules on teenage childbearing and dropout rates, among other things. The second project was a model of decision-making under uncertainty about future prices, as applied to marketing problems. The third is a model of investments in health over the life cycle. ■

Research Group and Collaborators

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Gautam Gowrisankaran, Associate Fellow

Estimating Hospital Quality Using a Bayesian Selection Model

In this project, Professor Gowrisankaran estimated the quality of care for pneumonia patients being treated by hospitals in Southern California, using Bayesian methods to control for patient selection based on severity of illness. The use of Bayesian methods has a number of advantages but is very computationally intensive. Because of the interactive nature of the Bayesian estimation algorithms, Professor Gowrisankaran was able to parallelize the computation.

This project sought to estimate the effects of competition for both Medicare and health maintenance organization (HMO) patients on the quality decisions of hospitals in Southern California. It was found that increases in the degree of competition for HMO patients decrease risk-adjusted hospital mortality rates. Conversely, increases in competition for Medicare enrollees are associated with increases in risk-adjusted mortality rates for hospitals. In conjunction with previous research, estimates indicated that increasing competition for HMO patients appears to reduce price and save lives, and hence appears to be welfare improving. However, increases in competition for Medicare appear to reduce quality and perhaps reduce welfare. The net effect of a given merger on hospital quality depends on the geographic distribution of different payer groups.

Another project concerned the causes and magnitudes of network externalities for the automated clearinghouse (ACH) electronic payments system, using a panel data set on individual bank usage of ACH. This researcher constructed a model of ACH usage to identify network externalities from correlations of increases in usage levels for banks within a network, and from increases in usage following exogenous increases in market concentration of size of competitors. He structurally estimated the parameters of the model by matching equilibrium behavior to the data, using simulated

maximum likelihood and a data set of localized networks. Estimation requires repeated computation of the equilibrium for different parameter values and values of the structural unobservables. Preliminary estimates reveal moderate network externalities that are principally due to lack of bank usage. Fixed costs of adoption are very variable across banks. Moderate subsidies to banks that adopt ACH are welfare improving. This study could potentially help shed light on the extent of any underuse of electronic payments technologies and other high-technology products. ■

Katherine Klink, Associate Fellow

Modeling Regional Climate-Vegetation Interactions During the Holocene in the Upper Great Lakes Region

Climate and vegetation in the Upper Great Lakes region (Minnesota, Wisconsin, and Michigan) have been influenced not only by continental-scale movement of air masses but also by substrate types and regional features such as the Great Lakes and the prairie-forest border. For a better understanding of Holocene climate-vegetation interactions in the Upper Great Lakes region, regional models of climate (RegCM2) and flora/vegetation (STASH AND FORSKA) were used to evaluate land surface-atmosphere interactions for the present day and for 11,000 (11k), 6k, and 3k years ago. Output from these models was linked to a pollen dispersion model (POLLSCAPE), and the results compared to observed fossil pollen from a high-quality, well-dated regional pollen database. The similarity of predicted and observed pollen assemblages were used to evaluate climate predictions. When disagreements occurred, their patterns in space and time helped to identify sources of error, and sensitivity studies continued to be used to evaluate the modeling strategies.

Another project involves the temporal and spatial characteristics of surface winds. Although the wind field is an important feature of the surface climate and is routinely reported by weather observers, little effort has been devoted to compiling a data set that describes these characteristics. This research focuses on temporal analyses of mean wind speeds and on measures of dispersion (such as variance and interquartile ranges). It involves using wind observations in the upper Midwest to evaluate the spatial and temporal variability in wind speed patterns. Some stations (e.g., LaCrosse, Wisconsin) show distinct periods of higher and lower wind speeds over the period, while other stations (e.g., Rochester, Minnesota) have a more or less monotonic upward trend in speed. There also is evidence that the statistical distri-

bution of wind speeds observed at several sites has changed over time, and this has implications for wind energy generation. ■

Diana Richards, Principal Investigator

Collective Choice With Shared Mental Models

Complex decision-making typically involves many agents attempting to aggregate many alternatives. Yet in these large collective choice settings, cyclic outcomes are highly probable, if agents' preferences are unconstrained.

In previous work, this research group showed that a knowledge-structure constraint on collective choice overcomes the aggregation paradox for small choice sets. Following this, the researchers expanded on these results to examine the probability of stable collective choice for large choice sets. The results will have implications for cognitive science, where an interpretation of sense data is made by aggregating information from a collective of brain modules; and for social choice, where a group decision is made by aggregating the preferences of a set of individuals.

Further studies will be performed concerning the probability of stable collective choice for large choice sets when players share a mental model of the choice context, as well as a study of the strategic manipulation of these mental models. Additionally, the researchers will study the effect of noise on the extent to which players agree on the mental representation of the choice set. ■

Research Group and Collaborator

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Shri Ramaswamy.....	68
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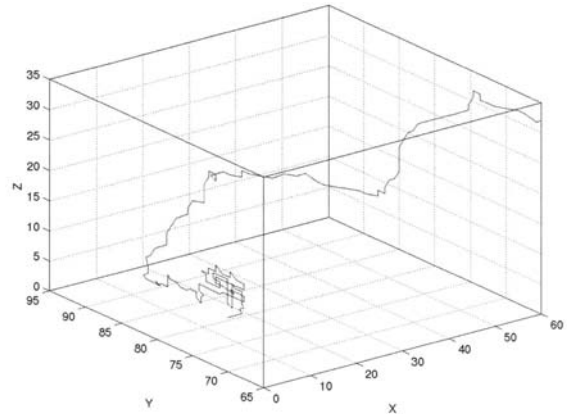
Shri Ramaswamy, Principal Investigator

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

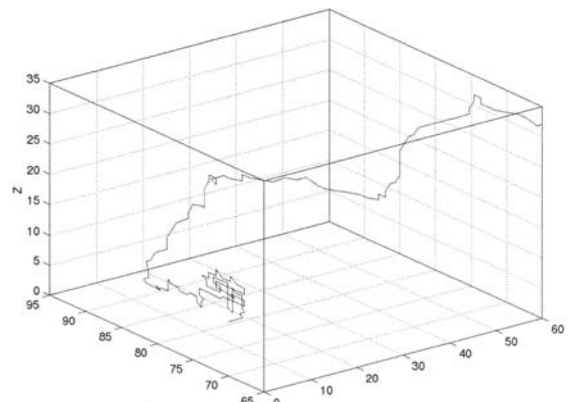
These researchers attempted to visualize and characterize the three-dimensional bulk structure of paper and board using non-intrusive techniques. Previously, they used laser scanning confocal microscopy (LSCM). This technique, although it is capable of non-intrusively visualizing paper samples, is limited by the depth or thickness that can be viewed. Further work using oil immersion lenses and LSCM showed that the quality of the images and interference from non-focal planes could be minimized. However, the researchers were still limited to a thickness of approximately 50 μm .

Explorations were performed with 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 were able to view the entire three-dimensional structure of thick (~300 μm) samples. These three-dimensional images were binarized (black and white) using methodologies developed by the group. This binarized image was then analyzed for pore structure characterization using supercomputing resources. 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. Also, numerical deconvolution of the three-dimensional images to sharpen the image, as well as to obtain better characterizations of the structure, will also be conducted using Supercomputing Institute resources.

Initial estimates of the structure characteristics indicate an immense potential for using this approach. Recent work using x-ray micro-tomography on paper samples of varying structure indicate that the technique is capable of visualizing the structure. The team's methods to characterize the internal pore structure revealed interesting information on the anisotropic nature of the internal structure. For



Trajectory followed by sample tracer through the pore structure in the in-plane direction.



Trajectory followed by sample tracer through the pore structure in the transverse direction.

example, measurements of tortuosity in the in-plane and transverse direction are very different with the transverse direction being more tortuous. This, along with other structural measurements, can explain the differences in transport properties in the in-plane and transverse directions. Efforts are underway in using higher resolution x-ray technique to get the finer details of the structure. ■

Research Group

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College of Pharmacy

Ramaiah Muthyala	70
------------------------	----

Department of Medicinal Chemistry

David M. Ferguson.....	71
Daniel M. Kroll	72
Philip S. Portoghese and Maria Germana Paterlini	73
W. Thomas Shier	74
Carston R. Wagner.....	75

Department of Pharmaceutics

David J. W. Grant.....	76
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Ramaiah Muthyala, Principal Investigator

Design of Anti-Viral and Anti-Cancer Drugs

This research is intended to develop designs for anti-viral and anti-cancer drugs using the following methods:

- Calculation of binding affinities of aspartyl proteases-ligand system (HIV—human immunodeficiency virus—inhibitors) by employing molecular dynamics and/or Monte Carlo simulations
- Conformational analysis of small molecules
- Modeling of G-protein coupled receptors ■

David M. Ferguson, Fellow

Simulation of Hairpin Loop Structures Using Molecular Dynamics; Modeling of Opioid Drug/Receptor Interactions

This group studies the structure, function, and dynamics of macromolecules and macromolecular interactions using a variety of computational techniques. These include molecular graphics, empirical force fields, *ab initio* calculations, molecular docking, and molecular dynamics simulations. A primary emphasis of this work focuses on the development and application of structural models of G-protein-coupled receptors (GPCRs) to ligand design. In particular, the researchers were concerned with developing highly selective opioid ligands with modified pharmacological properties. A second area of emphasis was placed on studying the structure, dynamics, and thermodynamic stability of modified nucleic acid complexes for use in antisense drug development. Both projects required significant force field parameterization, *ab initio* model calculations, and long time-scale molecular dynamics simulations, as well as graphics visualizations with the long-term goal of modeling molecular recognition processes reliably and confidently for use in drug design and development.

This group developed research on the conformations landscape of selective μ -opioid agonists in gas phase and in aqueous solution (the fentanyl series). Here, the conformational characteristics responsible for high affinity-opioid binding of a series of fentanyl analogs were investigated using a combination of molecular mechanics and molecular dynamics techniques. In general, the fentanyl analogs favor a conformation that is quite different in gas phase, and in the presence of explicit solvent or lattice packing forces. The most active analogs were shown to possess an extended conformation, while fentanyl derivatives displayed reduced binding affinities are predicted to favor compact arrangements. A superposition of the proposed "bioactive conformations" across this ligand series identified the orientation of the N-phenethyl and the N-phenyl group to be a con-

tributing factor responsible for the differential bind of the ohmefentanyl enantiomers, and other structural analogs. The 3-point pharmacophore model for the fentanyls also provided insights into the structure-activity relationship and served as a template for further QSAR and docking studies.

Deoxyribonucleic acid (DNA) hairpin loops are vulnerable spots on the DNA 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 been shown that this enzyme recognition is not entirely dependent on the sequence of the hairpin loop but is also believed to be dependent on the structure of the hairpin loop. Using molecular dynamics (MD) simulations, the researchers addressed 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 NMR studies have shown that the palindromic duplex sequence 5'd(CFCFTATATACFCF)3' is a dimer at lower temperatures and forms a hairpin loop structure at higher temperatures. Hence, the team studied this DNA hairpin loop structure using the AMBER code modules; they will analyze the structures obtained from their simulations in light of 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 that will provide new insights into the mechanism of DNA hairpin cleavage by nucleases. ■

Research Group

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Mesoscopic Models for Solvent Dynamics and Complex Fluids

In self-assembling fluids, correlated mesoscopic structures exist even far from critical points. This structure leads to anomalous scaling behavior in the dynamic structure factor as well as anomalies in the shear viscosity and the attenuation and dispersion of sound. In flow, the deformation of these correlated domains gives rise to excess stresses that result in rheological behavior that is quite different from that of simple Newtonian fluids. Near phase boundaries, shear can lead to dynamical instabilities and new structures in these systems. Similarly, flow-induced hydrodynamic stress on polymers or vesicles has a dramatic influence on both the shape of these networks as well as the rheology of suspensions. The objective of this project was to obtain a better understanding of the dynamics of complex liquids and the dynamical behavior of polymers and membranes in solvent. An essential component of this research was to develop and implement new algorithms based on generalizations of the lattice-Boltzmann method for the numerical simulation of the equilibrium and non-equilibrium dynamics to these systems. Unfortunately, the discrete nature of the velocity field in the lattice-Boltzmann approximation led to instabilities, which severely limit the usefulness of this method in a number of applications. This is particularly true when the method is extended to incorporate thermal fluctuations. For this reason studies were performed using a closely related mesoscopic model for solvent dynamics. This model utilized a synchronous, discrete-time dynamics with continuous velocities and local multiparticle collisions. The method is Galilean invariant, stable, and easy to implement on parallel architectures. Furthermore, all conservation laws were obeyed exactly, with fluctuations included. It can also be extended to model binary mixtures and more complex mixtures. The algorithms were developed for a wide range of applications in basic science and engineering.

The researchers are also continuing previous work on pore-scale simulations of dispersion. The group is performing a detailed simulation study of the scattering intensity at bulk and film contrast in microemulsion and sponge phases, in both symmetric and non-symmetric phases. The understanding of non-symmetric sponge phases is much less developed than that of the symmetric sponge phases the group has studied up to now. This work will lead to a better understanding of the internal structure of these phases and will allow the group to determine the scale dependence of the saddle splay modulus. Also, through comparison with neutron scattering data, this work will enable experimentalists to determine the values of the coarse-grained elastic constants of specific systems. ■

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Modeling of Opioid Receptors With Their Ligands

The transmembrane region of opioid receptors was reconstructed based on a previous structural template and recent experimental data on rhodopsin. The intracellular and extracellular loop regions were also modeled by these researchers. These regions, ranging from 9 to 25 amino acid residues in length, were studied using a previously developed conformational search algorithm for loops, together with indirect structural information obtained through site-directed mutagenesis data, secondary structure prediction and homology modeling. The models were then used to study the binding mode of both endogenous opioid peptides and alkaloids and to suggest possible mechanisms of receptor activation. Following this, the modeling effort was extended to predicting cross-linking of opioid receptors by affinity labels. Modeling results were used to propose a possible mode of interaction between these receptors and opioid ligands. ■

Research Group

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Transfection of PEI Derivatives

The use of polyethyleneimine (PEI) dendrimers as transfection vectors has shown promise compared to the use of traditional vectors such as viruses and liposomes. However, additional improvements will need to be made before these vectors can be used *in vivo* for human gene therapy. This research group is designing and synthesizing modified dendrimers with a polycation core. Around the core is a series of shells: first, a shell of hydrophobic chains, then a shell of acid (pH 5.0) cleavable linkers, and finally an outer oligocationic shell. The surface shell is intended to bind deoxyribonucleic acid (DNA) in the initial loading phase, but release it after the complex has entered the acid environment inside an endosome within the target cell. Computer-aided design is being used to estimate the size and density of oligocationic surface shell components that would both bind and release DNA efficiently. ■

Research Group

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Protein Dimerization

These researchers coupled two molecules of methotrexate via a methylene linker. Characterization of this compound indicated a highly folded conformation in an aqueous environment. Hydrophobic collapse and internal hydrogen bonding may provide the necessary stability for the methotrexate dimer's three-dimensional structure. By utilizing molecular modeling software, the researchers hoped to gain a grasp of the linker's contribution to the compound's solution structure and thus predict the effect that a change in the linker may have on the methotrexate dimer's folded structure. The folded structure of methotrexate, free of any linker, was also investigated. ■

Research Group

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Effects of Impurities Incorporated During Crystallization on the Crystal Properties of Some Therapeutic Agents; Effects of Salt Form and Crystal Habit on Tableting

Trace amounts of impurities present in the crystallization medium exert profound effects on the nucleation, growth, morphology, and properties of the crystals obtained. Structurally related impurities may be incorporated into the crystal lattice leading to changes in the crystal properties. These researchers set out to investigate:

- The effects of a diastereomeric impurity on the crystal properties of a chiral compound
- The influence of structurally related impurities on the stability of hydrates and on their solid-state reactivity
- The influence of crystallization conditions on impurity uptake and their subsequent effects on crystal properties of the host

The observed effects of incorporated impurities on the properties of the host were related to the molecular interaction in the solid-state between the host molecule and the impurity molecule. The molecular modeling tool was applied in these studies to view the crystal structures and hydrogen bond networks, and to calculate the lattice energy and intermolecular interaction energies.

A related area of study looked at trace amounts of impurities present in the crystallization medium. These exert profound effects on the nucleation, growth, morphology and properties of the crystals obtained. Structurally related impurities may be incorporated into the crystal lattice leading to changes in the crystal properties.

Another body of research developed by the researchers involved the effects of salt form and crystal habit on tableting. Tableting is an important yet very complex process in the pharmaceutical field. This project studied the effects of salt form and crystal habit on the tableting properties of some pharmaceutical

compounds. The CERUS2 program was employed for analyzing the crystal structure, and for calculating the attachment energy, theoretical powder x-ray diffraction patterns, crystal shape, crystallographic planes, and for identifying the slip planes, an important factor in the control of the mechanical (tableting) properties of powders.

These researchers also worked with eprosartan mesylate. This is used in the treatment of hypertension, and exists as an anhydrate, monohydrate, and dihydrate. The single crystal structures of the anhydrate and dihydrate were visualized and various interatomic distances and intermolecular energies were then calculated in order to assist in understanding, and ultimately in visualizing, the physicochemical properties and phase transitions of eprosartan mesylate. ■

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Department of Finance

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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 in this research avoids making detrimental assumptions. It facilitates empirical investigation of the shape of the market frictions and of the TS 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 the 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 by this group 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 the Canadian bond market. ■

William Li, Principal Investigator

Model-Robust Design and Non-Isomorphic Orthogonal Designs

This research project has two major objectives:

- 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.
- To construct complete catalogs of non-isomorphic designs. Orthogonal designs are 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.

While the former has received a great deal of attention in the literature, the latter has not been much discussed because the required computations are usually very large. Following recent articles by Ye and Li (2001) and Sun, Li, and Ye (2001), this research group uses a newly developed efficient algorithm and a theory based on the indicator function to construct complete sets of orthogonal designs with economic run sizes. ■

Research Group and Collaborator

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School of Public Health

Division of Epidemiology

James S. Pankow	81
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James S. Pankow, Principal Investigator

Genetic Epidemiology of Cardiovascular Disease and Associated Risk Factors

This research group seeks to detect, localize, and characterize genes involved in the development of cardiovascular disease (CVD) and its associated risk factors (i.e., diabetes, high blood pressure, elevated blood cholesterol, etc.). 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. For this reason, this group is using resources from the Supercomputing Institute. ■

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Department of Aerospace Engineering and Mechanics

Graham V. Candler.....	86
Roger Fosdick.....	87
Ashley James	88
Daniel D. Joseph	89
Perry H. Leo and John Lowengrub.....	91
Thomas S. Lundgren	92
Krishnan Mahesh	93

Department of Astronomy

Michael DuVernois.....	94
Thomas W. Jones	95

Department of Biomedical Engineering

Victor H. Barocas	97
-------------------------	----

Department of Chemical Engineering and Materials Science

Robert W. Carr	99
James R. Chelikowsky	100
Robert Cook	102
H. Ted Davis.....	103
Jeffrey J. Derby.....	104
William W. Gerberich	105
Wei-Shou Hu	106
Yiannis Kaznessis	108
Satish Kumar	109
Christopher W. Macosko	110
Richard B. McClurg.....	111
Alon McCormick	112
David C. Morse	114
Lanny D. Schmidt	115
L. E. Scriven	117
Renata M. Wentzcovitch	118

Department of Chemistry and Chemical Physics Program

George Barany	119
David A. Blank	120
Christopher J. Cramer	121
Mark Distefano	123
Jiali Gao	124
Thomas R. Hoyer	125
Steven Kass	126
Kenneth Leopold	128
Karin M. Musier-Forsyth	129
J. Ilja Siepmann	130
Donald G. Truhlar	133
Gianluigi Veglia	137
Darrin M. York	138

Department of Civil Engineering

Gary A. Davis	139
Robert J. Dexter	140
Catherine W. French and Carol Shield	141
Bojan Guzina	143
Miki Hondzo	145
Raymond Hozalski	146
Joseph F. Labuz	147
Joseph F. Labuz and Henryk K. Stolarski	148
Carol Shield	149
Henryk K. Stolarski	150

St. Anthony Falls Laboratory

Roger E. A. Arndt	151
Efi Foufoula-Georgiou	153
Fernando Porté-Agel	155
Charles C. S. Song	156
Heinz G. Stefan	157

Department of Computer Science and Engineering

Ding-Zhu Du	160
Vipin Kumar	161
Haesun Park	162
Yousef Saad	163
Jon Weissman	164

Department of Electrical and Computer Engineering

Anand Gopinath	165
James E. Holte	166
James Leger	167
David J. Lilja	168
P. Paul Ruden	170
Nikolaos D. Sidiropoulos	171
Randall Victora	172

Department of Geology and Geophysics

William Seyfried, Jr.	173
David A. Yuen	174

Institute for Mathematics and Its Applications

Fadil Santosa	177
---------------------	-----

School of Mathematics

Dennis Hejhal	178
John S. Lowengrub	179
Mitchell B. Luskin	181
Hans G. Othmer	182

Department of Mechanical Engineering

Avram Bar-Cohen	183
John C. Bischof	184
Jane Davidson	185
Sean C. Garrick	186
Steven L. Girshick	187
Richard J. Goldstein	188
Joachim V. Heberlein and Emil Pfender	189
Uwe R. Kortshagen	190
Thomas H. Kuehn and David B. Kittelson	191
Perry Y. Li	192
Benjamin Y. H. Liu	193
Susan C. Mantell	194
Peter H. McMurry	195
Suhas V. Patankar	196
David Y. H. Pui	197
Terrence W. Simon	198
Kumar K. Tamma	200
Michael R. Zachariah	201

Department of Physics

Charles E. Campbell	202
Cynthia A. Cattell.....	204
Eric Ganz	206
Alexander Grosberg	207
J. Woods Halley	208
Shaul Hanany	210
Norton M. Hintz	211
Robert L. Lysak	212
Oriol T. Valls	214

Graham V. Candler, Fellow

Simulation of Reacting Flows

This group has continued their research in the numerical simulation of high-temperature reacting flows. This work has several applications: supersonic flow control using laser energy deposition; generation of atmospheric-pressure air plasmas for materials processing and flow control; the study of how the Navier-Stokes equations fail in high-speed, low-density flows; the study of micro-scale aerodynamics; and the analysis of turbulent reacting flows. These researchers use a suite of computational fluid dynamics (CFD) codes developed for parallel supercomputers. These codes use implicit time integration to reduce the computational cost, and have been optimized for the IBM and SGI computers. This group also uses an efficient parallelized direct simulation Monte Carlo (DSMC) code for low-density flow simulations for comparison with the continuum CFD simulations. This work is leading to an improved understanding of how chemical reactions and fluid motion interact in a variety of technologically relevant applications. ■

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Dynamic Phase Transitions, Singularities, and Coexistent Phases in Elasticity

This group has continued its ongoing research on phase transitions, as well as investigating phases in elasticity. Purely mechanical theories of phase transitions require admissibility hypotheses—so-called “kinetic relations”—to be solvable. These kinetic relations, while ensuring uniqueness, have questionable physical justification. A thermomechanical model that includes capillarity, viscosity, and thermal conductivity is a more appropriate setting, and it is the preferred framework for this investigation.

In this setting, the idea is that the limiting solutions are physically relevant as the capillarity, viscosity, and thermal conductivity approach zero in a suitable manner. 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 showed that this is a promising method of calculating dynamic phase transitions. Further investigations, including the determination of dependence on numerical methods, were pursued.

This group implemented several finite difference and finite element methods for solving these equations, and they developed their own approach. Part of the difficulty concerns optimizing the computations and addressing the questions of parallelization and alternate numerical techniques.

This program of research also considered singularities in elastostatics. The nonlinear theory of elasticity is more promising for the investigation of coexistent phase phenomena and singular behavior in the mechanics of materials than its linear counterpart. 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 such nonlinear theories. Some of these ideas were used in these investigations, but the emphasis of this program has been on the role of singularities in problems where solutions are not regular. The injectivity of the deformation map was of major concern here.

Finally, the researchers began to develop a program to consider coexistent phases in non-local elasticity. The goal of this program was to carry out a theoretical and computational investigation of stable, equilibrium coexistent phase structures in solids when subject to external load, environmental temperature, or electrical simulation. The long-range plan adopted by these researchers was to turn to dynamical issues in this non-local theory. ■

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Ashley James, Principal Investigator

Numerical Simulations of Liquid-Fluid Interface Flows With Topological Transitions

Interfacial fluid flow is simulated to gain an improved understanding of how topological transitions of liquid-fluid interfaces occur. This group has developed an interfacial flow solver to investigate the use of vertical vibration to cause droplet ejection, and has submitted their research for publication. They are now working to modify the solver to improve its accuracy and extend its capabilities for the analysis of other physical systems.

Currently, a module to incorporate soluble surfactant is under development. This capability will be used to determine the effect of soluble surfactant on the break-up of a bubble in a shear flow. In another project, the code will be used to simulate the coalescence of two liquid drops. The method must be modified so that coalescence occurs selectively. The coalescence criterion will be based on a lubrication model of the fluid film between the two drops. Finally, the group is studying molecular dynamics simulations of interfacial breakup and coalescence with the aim of developing models of these processes for use in continuum-scale simulations. ■

Research Group

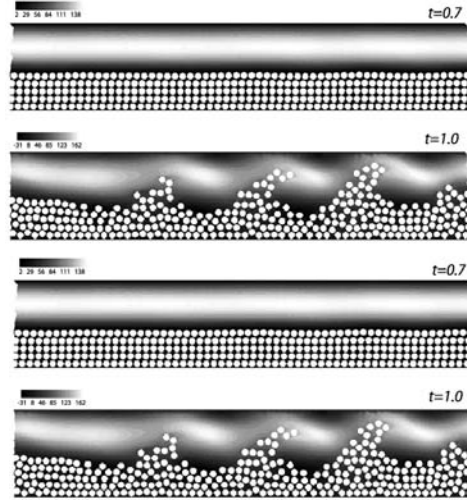
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Daniel D. Joseph, Fellow

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 researchers proceeded with their efforts to improve the performance of particle movers by developing improved preconditioners, and continued their computational investigations into the fundamental dynamics of fluid-particle motions. Work was conducted to develop models of the lift-off of particles from solid surfaces, which can then be used in making practical decisions in engineering applications, including sand transport in fractured oil reservoirs.

The researchers considered many specific topics within the field, one topic being the direct numerical simulation of solid-liquid flow. In direct simulation the fluid motion is resolved numerically and the forces that move the particles are computed rather than modeled. This procedure opens new windows for understanding and modeling. Numerical methods are discussed based on body-fitted moving unstructured grids and also on a fixed grid in which the portions of the fluid occupied by solids are forced to move as a rigid body by a



Lift-off of 300 heavy particles in a plane pressure-driven flow of a Newtonian fluid, $Re = 1,800$. Contour plot of the horizontal velocity component is shown. (Adapted from: N.A. Pantankar, T. Ko, H.A. Choi, and D.D. Joseph, “A Correlation for the Lift-Off of Many Particles in Plane Poiseuille of Newtonian Fluids,” *Journal of Fluid Mechanics*, 445, pp. 55–76 [2001].)

distribution of Lagrange multipliers. Animation of the fluidization of 1,204 spheres in three dimensions will be compared with experiments and the concept of fluidization of slurries in conduits by lift rather than drag will be framed in animation by direct simulation. Correlation for lift-off of single particles and the bed height of slurries fluidized by lift are obtained by processing data from numerical experiments.

Another study explored lift correlations from direct numerical simulation of solid-liquid flow. Lift forces acting on a fluidized particle play a central role in many important applications, such as the removal of drill cuttings in horizontal drill holes, sand transport in fractured reservoirs, sediment transport, and cleaning of particles from surfaces. This group studied the problem of lift using direct numerical simulations. They investigated lift formulas that respect the fact that the lift must change sign

Daniel D. Joseph, Fellow

on either side of the “Segré-Silberberg” radius and derived an accurate analytical expression for the slip velocity of circular particles in Poiseuille flow. The group has proven that the lift-off of single particles and many particles in horizontal flows follow laws of similarity, or power laws, which may be obtained by plotting simulation data in two dimensions on log-log plots. For the first time, they have processed data from slot experiments on bed erosion for fractured reservoirs in log-log plots. The research results showed that power laws with a parameter dependent power emerge as in the case of Richardson-Zaki correlations for bed expansion. ■

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

This research group continues its investigation of microstructures formed in crystalline alloys using a dual approach with sharp and diffuse interface methods. A main focus of this study is to develop a three-dimensional sharp interface model to study equilibrium shapes, morphological instabilities (particle splitting), and multi-particle coarsening. A secondary focus will be to include multi-component diffusion, multiple phases, and kinetics in both diffuse and sharp interface models. These features are needed to include solid-state reactions in the transformation models.

A past study conducted by this research group demonstrated that a morphological instability driven by deviatoric applied stresses can generate elastically-induced particle splitting. The splitting occurs when the elastic fields are above some critical value. Below this value one observes a small perturbation consistent with the splitting, but the perturbation is stabilized by surface tension. Ongoing work includes developing a three-dimensional boundary integral method to track precipitate motion. Progress has been made in finding equilibrium shapes for three-dimensional particles and investigating the morphological stability of a particle. In particular, the group has found that concave shapes can be generated by external fluxes; these shapes may lead to particle splitting as described above. ■

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PDF For Turbulent Flow

This research centered on the deformation and breakup of liquid drops in high-speed gas streams by means of boundary integral numerical methods. The application sought to demonstrate the secondary breakup of fuel spray droplets in high-pressure gas turbine combustion chambers.

The researchers also developed a new method for closing the equation for the probability density function (PDF) for isotropic, homogeneous turbulent flow. This first order partial differential equation in six variables, plus time, is a generalized Boltzmann equation, which can be solved by numerically integrating its characteristic equations backward in time to the intersection with initial specified data. The method of closure along with the solution method ensured that the PDF remains positive. ■

Research Group

Ram Rao, Research Associate

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. Large-eddy simulation 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 equations (RANS). LES is, however, more computationally intensive. Also, LES has traditionally been restricted to simple geometries, such as channels, backsteps, mixing layers, jets, etc. 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, and 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.

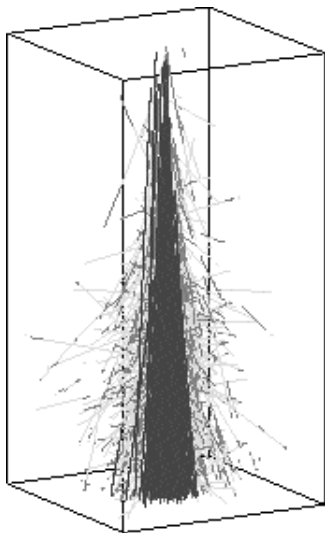
Such robustness is imperative to perform accurate simulations in complex geometries at high Reynolds numbers. The primary goal of this research was to develop the capability to perform LES in configurations relevant to industry. ■

Research Group

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Michael DuVernois, Principal Investigator

Simulations of High-Energy Cosmic-Ray Air Showers



The Pierre Auger Observatory, under construction in Western Argentina, observes cosmic-ray air shower cascades, which can exceed 10^{20} eV and 10 billion secondary particles. A University of Minnesota School of Physics and Astronomy group is active in both the construction of the detector and large-scale simulations of the air shower physics.

The principal method of studying extremely high-energy cosmic rays is to study the properties of the shower of particles resulting from the initial impact with molecules in the atmosphere. Such showers of secondary particles (which can number in the billions) are typically simulated with two software packages: MOCCA, an older FORTRAN code with a long history of comparisons with theory, and AIRES, a modern FORTRAN and C code with updated physics. In support of the Pierre Auger cosmic-ray observatory, currently under construction to observe the highest energy cosmic rays ($E > 10^{20}$ eV), this group is studying the parallelization and optimization of MOCCA and AIRES for large-scale simulations aimed at producing a standard shower library for the experiment.

As one component of the air-shower simulation work of the Pierre Auger Observatory, this group migrated the existing air shower simulation toolkits MOCCA and AIRES to the IBM SP and SGI Origin at the Supercomputing

Institute. This included studies of the serial use of the air shower simulation code as well as a message passing interface-based multiprocessing implementation of the software. This work provided a potential high-speed environment for producing large numbers of sample air showers to form a library for use in detector calibration efforts. ■

Research Group

Chihwa Song, Research Associate

Thomas W. Jones, Fellow

Numerical Studies of Particles and Fluids in Astrophysics

These researchers continued their pioneering effort in the study of the acceleration and propagation of high-energy charged particles in cosmic plasmas, as well as some key associated astrophysical phenomena. Three large groups of magnetohydrodynamical (MHD) simulations that include innovative treatments of particle transport and other novel approaches were proposed. This group has applied their methods to the study of giant radio galaxies powered by the propagation of hypersonic plasma jets, to simulations of large-scale cosmological structure formation associated with clusters of galaxies, and to supernova remnants, the hot, chaotic bubbles formed when exploding stars blast through the diffuse interstellar medium. Since the researchers alone have the computational tools to model these phenomena in this level of physical sophistication, and since these problems are all fundamental to astrophysics, the simulations were expected to be extremely important. Each of the projects conducted by this group provides the core material for a Ph.D. thesis in progress.

One specific project performed by this research group involved simulating electron transport and synchrotron emission in radio galaxies. In this study, the researchers developed the first three-dimensional MHD radio galaxy simulations that explicitly model transport of relativistic electrons, including diffusive acceleration at shocks as well as radiative and adiabatic cooling in smooth flows. Three simulations of light Mach 8 jets, designed to explore the effects of shock acceleration and radiative aging on the non-thermal particle populations that give rise to synchrotron and inverse-Compton radiations, were investigated. Because the goal of this project was to explore the connection between the large-scale flow dynamics and the small-scale physics underlying the observed emissions from real radio

galaxies, the researchers combined the magnetic field and relativistic electron momentum distribution information to compute an approximate but self-consistent synchrotron emissivity and produce detailed synthetic radio telescope observations.

Several key insights have surfaced from this approach:

- The jet head in these multidimensional simulations is an extremely complex environment. The classical jet termination shock is often absent, but motions of the jet terminus show a “shock-web complex” within the backflowing jet material of the head.
- Correct interpretation of the spectral distribution of energetic electrons in these simulations relies partly upon understanding the shock-web complex, for it can give rise to distributions that confound interpretation in terms of the standard model for radiative aging of radio galaxies.
- The magnetic field outside of the jet itself becomes very intermittent and filamentary in these simulations, yet adiabatic expansion causes most of the cocoon volume to be occupied by field strengths considerably diminished below the nominal jet value. Radiative aging is very slow in these volumes, so population aging rates vary considerably from point to point.
- Overall, the intricate dynamical behaviors in these models make it difficult to capture the histories of the non-thermal particles in broad generalizations. Understanding even the simplest of these models requires attention to details of the flow. ■

Research Group and Collaborators

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Victor H. Barocas, Principal Investigator

Simulation of Controlled Intraocular Drug Delivery

The vitreous and retina—the two primary components of the posterior eye—are particularly difficult to treat with pharmaceutical agents because of poor access by standard delivery techniques. Systemic delivery is impeded by the blood-retinal barrier, topical delivery via eyedrops is prone to washout by the tear film and aqueous humor, and repeated direct intraocular injection is understandably unattractive to many patients. As a result, controlled release systems—such as drugs entrapped in degradable polymers or micropumps attached to drug reservoirs—have emerged as an alternative. Determining the optimal location and delivery rate from the source is a problem that requires three-dimensional simulation of the release, transport, and kinetics of the drug.

This group expected to develop a preliminary model for release from a point source at a set location. This projected work would include techniques being developed in the lab of T. W. Olsen of the Department of Ophthalmology.

At the same time, the research group expected to work on two high-performance computing projects within the area of computational biomechanics. The first project was to deal with coupled mechanics of the Newtonian fluid comprising the aqueous humor, and the iris, an elastic solid, in the anterior portion of the eye. Having previously developed a two-dimensional simulation of this system that can play an important role in certain forms of glaucoma, the researchers looked forward to extending their model to three dimensions. While they would focus on two specific, three-dimensional problems—changes to the aqueous humor flow field when a hole is burnt into the iris by a laser and coupled heat and momentum transfer in the aqueous humor due to evaporative cooling of the cornea—the research group also would seek a novel macroscopic-microscopic finite element approach to the modeling of fibrillar tissues. This approach, although computation-

ally intensive, should offer the potential to provide much more insight into the mechanical behavior of tissues and tissue equivalents, as formed by cells entrapped in a reconstituted biogel. Having demonstrated the effectiveness of their approach on a test problem using workstations, the researchers looked forward to studying real systems, and to performing their work using much greater mesh refinement in three dimensions.

One specific research project conducted in this area over the past year involved a Boussinesq model of natural convection in the human eye and the formation of Krukenberg's spindle. Here, the cornea of the human eye is cooled by the surrounding air and by evaporation of the tear film. The temperature difference between the cornea and the iris (at core body temperature), causes circulation of the aqueous humor in the anterior chamber of the eye. Others have suggested that the circulation pattern governs the shape of the Krukenberg spindle, a distinctive vertical band of pigment on the posterior cornea surface in some pathologies. These researchers modeled aqueous humor flow in the human eye, treating the humor as a Boussinesq fluid and setting the corneal temperature based on infrared surface temperature measurements. The model predicts convection currents in the anterior chamber with velocities comparable to those resulting from forced flow through the gap between the iris and lens. When paths of pigment particles are calculated based on the predicted flow field, the particles circulate throughout the anterior chamber but tend to be near the vertical centerline of the eye for a greatest period of time. Further, the particles are usually in close proximity to the cornea only when they are near the vertical pigment spindle.

Another study conducted by this research group dealt with coupled macroscopic and microscopic scale modeling of fibrillar tissues and tissue equivalents. Collagen mechanics are

Victor H. Barocas, Principal Investigator

crucial to the function and dysfunction of many tissues, including blood vessels, articular cartilage, and bioartificial tissues. Previous attempts to develop computer simulations of collagenous tissue based on macroscopic property descriptions have often been limited in application by the simplicity of the model; simulations based on microscopic descriptions, in contrast, have numerical limitations imposed by the size of the mathematical problem. This method combines the tractability of the macroscopic approach with the flexibility of the microstructural approach. The macroscopic domain is divided into finite elements (as in standard finite element method). Each element contains a microscopic scale network. Instead of a stress constitutive equation, the macroscopic problem is distributed over the microscopic scale network and solved in each element to satisfy the weak formulation of Cauchy's stress continuity equation over the macroscopic domain. The combined method scales by order 1.1 as the overall number of degrees of freedom is increased, allowing it to handle larger problems than a direct microstructural approach. Model predictions agree qualitatively with tensile tests on isotropic and aligned reconstituted type I collagen gels. ■

Research Group

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Atmospheric Chemistry of the Chlorine-Containing Organic Compounds

Supercomputing Institute resources were used to complement experimental research on atmospheric chemistry of halogenated alkoxy radicals and the chemistry of GaN chemical vapor deposition. By performing *ab initio* calculations on reactions of CF_3CClHO , $\text{CF}_3\text{CH}_2\text{O}$ and CH_2BrO radicals, the researchers predicted optimized geometries, vibrational frequencies, and total energies of reactants, products, and transition states. Reaction path following calculations will also be used to verify that the located transition states connect with two minima in each side of the reaction coordinate (reactant and products). The results of the *ab initio* computations will be used in Rice-Ramsperger-Kassel-Marcus (RRKM) estimates of rate coefficients via molecular theories of kinetics. Comparisons were made between the computations and experimental results. Comparison of the estimated and experimental rate coefficients permit 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.

One study involved an *ab initio* molecular orbital study of the unimolecular elimination of HCl and Cl from the CH_2ClO radical.

Geometry optimizations were carried out at the HF/6-31G(d), MP2(full)/6-31G(d), and MP2(full)/6-31G(d,p) levels, and total energies were calculated using G2 and G2(MP2) theories. The zero point energy (ZPE)-corrected energy barrier for HCl elimination is predicted to be 8 kcal/mol, and for Cl elimination it was predicted to be 10.5 kcal/mol. RRKM models for both unimolecular reactions were made from the *ab initio* vibrational frequencies (scaled), moments of inertia, and barrier heights. The RRKM predicted thermal rate

coefficients for HCl elimination are in good agreement with experimental data taken over the temperature range 265–306 K and the pressure range 5–35 torr (Wu and Carr, *J. Phys. Chem. A*, 105, p. 1423, 2001) when the barrier height is adjusted to 8.5 kcal/mol. Because of the low energy barrier and, to a lesser extent, the small size of the reactant, the fall-off curve is very broad, and the high pressure limit is predicted to be closely approached only when pressures of 107 torr and above are reached.

A second research project conducted by this research group investigated homogeneous gas phase reactions that occur during chemical vapor deposition (CVD) of GaN from NH_3 and trimethylgallium (TMG). Both experimental and theoretical studies are necessary to develop a physically based detailed CVD reactor model for GaN deposition. For the first half of 2002, these researcher will study the successive loss of CH_3 radicals from TMG, and decomposition of TMG:NH_3 via *ab initio* and RRKM methods. ■

Research Group

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High-Performance Algorithms for Electronic Materials

This research group has 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 and novel 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 has also initiated a new program on dilute magnetic semiconductors.

These researchers explored *ab initio* absorption spectra and optical gaps in nanocrystalline silicon. The optical absorption spectra of Si_nH_m nanoclusters up to ~250 atoms were computed using a linear response theory within the time-dependent local density approximation (TDLDA). The TDLDA formalism allows electronic screening and correlation effects, which determine exciton binding energies, to be naturally incorporated within an *ab initio* framework. Calculated excitation energies and optical absorption gaps of this project were in good agreement with experiment in the limit of both small and large clusters. The TDLDA absorption spectra exhibited substantial blueshifts with respect to the spectra obtained within the time-independent local density approximation.

Ab initio calculations for structure and temperature effects on the polarizabilities of Na_n ($n \leq 20$) clusters have also been examined by this group. They performed a rigorous, *ab initio* theoretical calculation of the dependence of Na cluster polarizability on cluster size, up to 20 atoms, obtained by combining *ab initio* pseudopotentials with a gradient-corrected density functional. Using molecular dynamics, it was found that for clusters as small as nine atoms, a multitude of degenerate isomers exists

even at $T = 0$. By calculating the polarizability of these isomers, these researchers reproduced the generally decreasing nature of the measured polarizability curve, as well as its dips at “magic” numbers corresponding to closed electronic shells. Moreover, they found that the effect of a finite temperature on the cluster structure suffices to account for most of the quantitative discrepancy between theory and experiment.

These researchers, in collaboration with workers from the National Institute of Standards and Technology (NIST), have developed an experimental method by which site-specific valence-electronic structure may be obtained. It uses the spatial dependence of the electric-field intensity that results from the superposition of the incident and reflected x-ray beams within the vicinity of a crystal x-ray Bragg reflection. The researchers demonstrated resolution of the anion and cation contributions to the GaAs valence band and compared it to an *ab initio* theoretical calculation of the Ga and As partial density of states.

In another area of research, structural and electronic properties of Cd_nX_n ($\text{X}=\text{S}, \text{Se}$; $n=2-8$) were calculated using the finite-difference pseudopotential method in real space. The computed ground state atomic configurations for the Cd_nX_n clusters deviate substantially from those for Si_{2n} and Ga_nAs_n . The increased ionic character of the bonding in Cd_nX_n clusters accounts for the observed structural variations. By calculating the highest occupied molecular orbital–lowest unoccupied molecular orbital gaps, binding energies, and polarizabilities of the clusters, this team found a strong correlation between the binding energies and gaps. The computed polarizabilities for the (CdS, CdSe) clusters follow the same trend with size as for Si and GaAs. The polarizabilities rapidly approach the bulk limit from above for clusters with more than ~10 atoms. ■

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Slitting of Coated 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:

- Thin polymer films coated with magnetic materials that are slit to form magnetic recording tape
- Thin polymer films coated with optically-sensitive emulsions that are slit and punched to form photographic film
- Paper multi-layer structures that are slit, cut, and punched to form adhesive labels
- Metal-coated polymer-ceramic composite sheets that are cut and punched to form multilayer chip capacitors or semiconductor substrates

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. They include "slitting" models (two-dimensional and three-dimensional) with different cutting mechanisms (e.g., mode-III fracture, plastic flow, etc.), a mode III fracture model to simulate the crack in the magnetic supported layer, and a plane-strain mode-II "sliding" fracture model to study delamination. Explicit quasi-static analysis will be performed for some of the proposed "slitting" models. Elastic and viscoelastic material laws will be used in these models.

The project also includes testing of the different mechanical, fracture, and adhesive properties of the films to be studied. ABAQUS finite element models will also be used to complement the experimental work. In particular, a three-dimensional model of time-dependent deformation will be developed to describe depth-sensing indentation ("nanoindentation") of multiplayer magnetic tapes. The models will allow elastic, plastic, viscous, and densification properties of the top, data storage, layer of the tape to be deconvoluted from load-displacement responses of the entire tape stack, and will provide insight into the contact mechanisms of porous materials. ■

Collaborator

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H. Ted Davis, Fellow

Fluid Physics for Technologies

These researchers used Supercomputing Institute resources to investigate fluid physics and associated phenomena underlying current and future process technologies. A concomitant to this research was the development of efficient computational mathematics and numerical methods for the problems and machines at hand. The problems are typically nonlinear and multidimensional, often involving coupled partial differential and integral equations, and also frequently have time dependence. The mathematical methods principally employed include:

- Subdomains, adaptive sub-domaining, and finite element basis functions
- Isoparametric mapping into a computational domain
- Newton iteration with continuation
- Vectorized calculation of the coefficients of basis functions (adaptive time-stepping and iterative diagonalization of large Hermitian matrices)

Usually the structure of the solution space—folds, bifurcations, etc.—that is, the number of solutions and their stability—is much more important than individual solutions. Most of the problems are not excessively large but have to be solved many times to map solution space. Transient behavior is often important and typically multiplies by two orders of magnitude the number of times the basic problem must be solved. The problems are usually highly vectorizable.

This team is also developing parallel computer methods for simulating the interior region of a liquid chromatographic column. A detailed flow field is developed from a pore-scale calculation of low Reynolds number flow in a packed bed of surface-retentive particles. The fluid-mechanical calculations are performed with a lattice-Boltzmann technique.

Convection, diffusion, and retention of a solute are modeled by stochastic algorithms based on

the Langevin equation. The computational scheme offers the ability to reproduce essential dynamics of the chromatographic process from fundamental considerations of packed bed geometry, flow velocity, solute diffusivity, and adsorption parameters. ■

Research Group and Collaborators

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Materials Processing Fundamentals

Large-scale numerical modeling is employed to study several materials-processing systems. On the continuum level, these systems are characterized by non-linear interactions between field and inter-facial phenomena. These phenomena—specifically, the transport of momentum, heat, and mass and effects of solidification and capillarity—are analyzed via finite element computations.

On the atomistic level, this research group performed *ab initio* simulations (in collaboration with James Chelikowsky, Department of Chemical Engineering and Materials Science) 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. The current work focuses 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.

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 modeling vacancy diffusion phenomena, which dominate the sintering behavior of crystalline materials, and extending analyses to more complicated, three-dimensional particle arrangements.

The researchers are also developing methods to describe microwave heating. They have developed finite element techniques to study the microwave heating of solids and liquids in various materials processing systems, and are studying food processing.

Lastly, the team is studying polymer fluid dynamics in processing. The researchers are developing and applying finite element methods with differential constitutive equations for viscoelastic fluids to study various flows in polymer processing. Of particular interest are polymer drop deformation and break-up in extensional and shear flows. ■

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

The purpose of this research was to develop an efficient model for micro- and nanoindentation of solidified/solidifying polymeric coatings and to probe mechanical properties of polymers with both nanoindentation technique and the model. In the previous stage of this research, two- and three-dimensional explicit finite difference models of elasto-plastic micro- and nanoindentation and microscratch with large deformation were developed and run successfully on the Crays.

Most recently, this research was extended to the modeling of micro- and nanoindentation of viscoelastic polymers using specially developed code on the SGI Origin 2000 and IBM SP. The model was applied to relaxation and creep responses in viscoelastic nanoindentation. Three kinds of indenters are of interest to these researchers: strip, flat-ended cylindrical, and spherical. It was expected that the model would consider both compressible and incompressible polymeric coatings, and that this model would assist in applying nanoindentation technique to data acquisition of viscoelastic materials more efficiently. ■

Research Group

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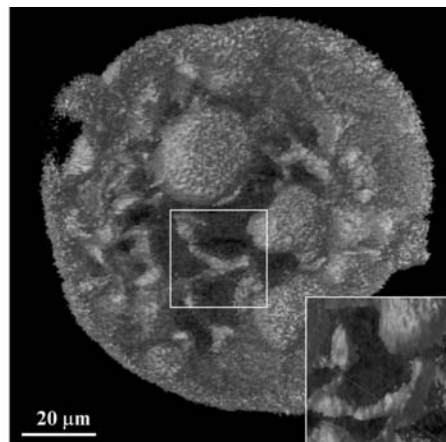
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Mechanistic Study of Hepatocyte Spheroid Formation; Modeling Regulatory Networks and Cell Metabolism From a Global Perspective

The study of tissue formation *in vitro* requires the use of noninvasive tools. To that end, these researchers used confocal microscopy in conjunction with image analysis to observe the mechanical behavior of hepatocytes during their self-assembly in round aggregates or spheroids and to probe their functions within these three-dimensional structures. The out-of-focus information—as well as the electronic noise introduced during image acquisition—can result in artifacts and impede further data analysis and volume reconstruction. Subsequently, the processed images were transferred for three-dimensional reconstruction to the SGI workstations in the Basic Sciences Computing Laboratory (BSCL).

In this work, the group developed an assay, which requires the use of confocal microscopy and image analysis, for *in situ* assessment of CYP2B1/2 activity in three-dimensional tissue-like structures of primary hepatocytes. The images taken at different time points and the subsequent reconstruction revealed the spatiotemporal bioactivity of hepatocytes in the aggregate. The visualization of cellular and subcellular activities during the formation of tissue-like structures is crucial in elucidating aspects of the mechanisms that cells employ during these phenomena. Better understanding of these phenomena has a great impact in tissue engineering and drug screening applications.

The different states during the course of spheroid formation are characterized by differing patterns of gene expression. With the dramatic progress in sequencing the genomes of different organisms, it is now possible to monitor the expression levels of all the genes in the genome simultaneously. One of the promising methods is carrier deoxyribonucleic acid (cDNA) microarray analysis of gene expression profiles. In this process, labeled cDNA is incubated on a DNA microarray containing thousands of spots, each corresponding to a unique



Self-assembled hepatocyte spheroids with internal channels.

DNA sequence. It is assumed that the fluorescence intensity of a spot is proportional to the initial concentration of the corresponding cDNA species 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.

The research team has developed a kinetic model for the hybridization process that considers the dynamics of diffusion of labeled cDNA strands and duplex-formation reactions. They used finite element analysis to numerically solve the partial differential equations that arise from the modeling. This study's goal 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 defined concentration and identity of labeled cDNA species.

Another project by this group involves modeling regulatory networks and cell metabolism from a global perspective. Cell metabolism is essentially a complex network of reactions with many enzymes and reactants involved, as well as a regulatory network controlling the expres-

sion 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, including physiological, differentiation, and developmental, involve the interplay of these regulatory networks.

Models of cell metabolism provide a deeper understanding and a way to organize these reactions and the interactions that occur inside cells. Dynamic models additionally provide a way to study and predict the behavior and changes over a time period that cells experience when exposed to environmental changes. This knowledge provides an essential link between functional genomics and physiomics. With the advent of the post-genomic era, a variety of large-scale gene expression profiling techniques, such as DNA microarrays, has enabled this group to survey the temporal expression pattern of the regulatory elements. Deciphering this information for reconstructing the hierarchy of the regulatory elements is becoming even more urgent.

There are several possible approaches for modeling regulatory elements. This group developed an algorithm based on the Boolean framework to reverse engineer the network. A set of parsimonious networks is predicted from expression profiles obtained by perturbing the network under different conditions. Computational simulations have been presented to substantiate these results. The group evaluated the performance of the proposed algorithms using both a set of synthetically-generated networks as well as an actual network such as that derived from the yeast cell mating pathway. The group generated a set of synthetic networks by varying the number of genes/nodes, connections/edges, and maximum degree of a node. Both acyclic and cyclic networks were considered. For each node, the researchers used a randomly-generated con-

junctive expression to generate its Boolean function. Care was taken to ensure that the gene would not be independent of its immediate inputs. Using this approach, the group generated a number of different networks with genes varying from 10 to 100 and with varying in-degree. The programming is done entirely in c. However, exploring the entire possible network space demands many computer resources and the problem quickly scales up with the number of nodes.

The number of equations and reactions required to describe cell metabolism is large, due to the number of enzymes and reactions that are involved in this complex network. This modeling approach tends to reduce the number of equations used to accurately describe cell metabolism. First, the network is identified. Kinetic expressions based on mechanistic knowledge are used to describe each reaction. Then, the system is simplified based on the differences in time scale where each of these reactions occurs. This provides a systematic way to analyze and describe these systems and to properly examine steady-state assumptions (that are usually made for fast reactions) without eliminating the effect that the fast reactions have on the slower reactions and the whole metabolic network.

This approach requires the use of symbolic computation methods (like MAPLE or MATHEMATICA) for the analysis of the network, determination of constraints derived from the faster-scale reactions, simplification of the differential algebraic equations, and numerical solution of the simplified system. ■

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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 the 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, the problem of 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, this research group is investigating the morphology of monolayer films of dipalmitoylphosphatidylcholine (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. ■

Satish Kumar, Principal Investigator

Gravure Coating and Printing Technologies

Gravure coating and printing are processes that are capable of producing thin coatings or fine patterns on substrates at high speeds by using a cylinder engraved with grooves (for coating) or cells (for printing). Gravure technology is already well established, but the controlling phenomena are not adequately documented. A complete understanding of the flow in gravure grooves and cells is vital for the prediction and optimization of coating and printing processes.

In gravure operations, the engraved cylinder is often used in conjunction with a smooth deformable cylinder in order to get thinner coatings and to avoid wear of the engraved cylinder's surface. These researchers' objective is to model the flow between a gravure groove/cell and a deformable roll. Because the gap between the two cylinders is usually so small that the flow is essentially one-dimensional, lubrication theory may be applied. The pressure distribution in the gap is governed by a very stiff nonlinear ordinary differential equation (ODE), whose solution requires special integration algorithms. Previous work by others on similar ODEs indicates that the International Mathematical and Statistical Library routine `DGEAR`, a variable-order predictor-corrector method, is suitable for solving such stiff systems.

The results of the calculations this group is running on the Supercomputing Institute's workstations will yield information about how pressure distribution, flow rates, and surface separation profiles in the cylinder gap depend on groove/cell geometry. This information can then be used to optimize groove/cell design, something that is of great interest to companies engaged in gravure operations. The results obtained with the simplified model will be compared to observations obtained from flow visualization experiments, as well as to more detailed finite-element calculations. ■

Research Group

Xiuyan Yin, Graduate Student Researcher

Christopher W. Macosko, Associate Fellow

Modeling Area Generation in Polymer Binding

Recent experimental work has revealed that viscoelastic drops suspended in another viscoelastic medium tend to flatten considerably when exposed to shear flow. This mode of area generation holds potential as a means for more easily creating polymer barrier materials, among other possible applications. An exploration of this phenomenon, from a fluid dynamics approach by solving the governing transport equations using the Finite Element Method (FEM), was the next step in this group's research trajectory.

The key features and challenges of the problem included the following: full three-dimensionality; two phases, one or both phases being viscoelastic; time-dependent flow; and the drop shape defined by a moving boundary. While FEM is ideally suited to such a problem, difficulties arise in choosing or developing a numerically stable variation of FEM, which allows for large departures from Newtonian fluid behavior. In addition, the three-dimensional aspect of the problem requires special attention to deal with problem size and computation time.

The research team has developed code for extending the FEM used previously to study viscoelastic drop formations in symmetric flows to fully three-dimensional flows. They have incorporated adaptive remeshing into the algorithm to allow very large drop deformations to be tracked. Complex phenomena such as many-body effects, e.g. flow-induced collision and coalescence of deformed drops, have been included in the simulations. This research is being extended to include inertial effects, coupled heat and mass transfer, and effects of surfactants on the deformation and coalescence of drops. ■

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Intermolecular Potentials Inferred From Crystallographic Data

Prediction of molecular crystal structures is extraordinarily difficult due to the extreme sensitivity of the free energy surface to small changes in the intermolecular potential. This research group is using this sensitivity to their advantage by inverting the problem. Given observed crystal structures, they are working towards inferring constraints on intermolecular potentials that are consistent with the observations. Due to the extremely sensitive dependence of crystal structure on intermolecular potentials, these constraints define a very small family of candidate potentials.

As a starting point, this group is modeling tetrahedral molecules that form “plastic” crystals. Plastic crystals are orientationally disordered at high temperature, but have ordered phases at low temperature. The group has used the Cambridge Structural Database to identify structures and phase transitions for a group of tetrahedral plastic crystals (e.g., carbon tetrabromide, adamantane, silane, etc.), which will serve as a test case. They are modeling the intermolecular potential using a generic Fourier expansion of orthogonal symmetry-adapted rotator functions are developing methods for inferring constraints on the Fourier coefficients using the structural and phase transition information. This is part of an ongoing effort to establish the relationship between intermolecular potential and crystal structure. ■

Research Group

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Modeling of Linear Viscoelasticity; Molecular Scale
Chemical Reaction Engineering of Materials Synthesis;
Visualization of Sorbates in Zeolite Pores

Free-radical polymerization of multifunctional monomers such as (meth)acrylates lead to the formation of highly crosslinked polymer networks. These networks have found applications in coatings, films, information technology, and other areas. However, such crosslinking polymerization exhibits special features that 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 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 which incorporates the connectivity of the entire network. The equation governing the stress development is then given by a differential algebraic equation (DAE), which can then be solved to obtain changes in the stress state of the system with time. The model’s results have provided valuable insight into viscoelasticity in a network.

A network of springs and dashpots can also be used for modeling curing coatings. The liquid monomer is represented by a network of dashpots. As the reaction in the network takes place, a dashpot is replaced with a spring as bonds start forming. Thus, elasticity in the network builds up 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 also allow the group to optimize the curing process in order to maximize the conversion and minimize stress.

Studies have also been started to understand wrinkling of coating surfaces. This will involve modeling of stress in the coating and some instability studies for the coating surface.

Molecular simulations have been a potent tool in studying the behavior of molecules in nano-confined spaces—in small- and medium-pore zeolites, for example. They have been used to study mobility of the molecules, their adsorption dynamics, and separations based on the above-mentioned behavior, all of which may be very different from what one would expect from their bulk properties. In the past, simple spherical molecules or those that could be approximated reasonable as spheres were studied. This group has begun to look at aromatics, a set of molecules with complex geometry, to learn about their packing behavior, mobility, and adsorption dynamics using molecular dynamics and Monte Carlo simulations.

The group used simulations of adsorption of shaped molecules in zeolite pores of different types to identify certain principles of shape selectivity. The next step in this research will be to study how shaped molecules diffuse differently in zeolite pores. The group hopes to be able to use the results of these studies to develop separation techniques for these compounds—a very important, economically-driven need for the petroleum and petrochemical industry. Also, the group hopes to learn enough from this research to develop a technique for economical, good separation of similar compounds used by the pharmaceutical and specialty chemical industries. ■

Research Group

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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 application of this research program, the group studied the linear viscoelasticity of dilute solutions of semiflexible polymers, by means of Brownian dynamics simulation and theoretically. The shear relaxation modulus $G(t)$ for chains that are shorter than their persistence length exhibits three time regimes: at very early times, when longitudinal deformation is affine, $G(t)$ and the tension both decay; over a broad intermediate regime, during which the chain length relaxes, $G(t)$ decays as $t^{-5/4}$; at long times, $G(t)$ is similar to that of rigid rods.

The researchers have completed initial tests of the first working version of 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 periodic 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. ■

Research Group

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Two-Dimensional Reactor and Catalytic Radiant Burner Modeling Using Detailed Chemistry

High-temperature, short contact time catalytic reactors show great promise in many applications, ranging from the production of synthesis gas and olefins to catalytic combustion and incineration. These researchers studied the production of oxygenates and olefins from the partial oxidation of alkanes in a single-gauze reactor and the production of high concentration hydrogen syngas streams from partial oxidation of methane in monolith reactors with steam addition. This project focused on the detailed fluid dynamics and reaction pathway simulations associated with these reactors.

The oxidation of cyclohexane over a Pt-10% Rh single-gauze catalyst was carried out in the laboratory. This process enables the exothermic production of an outlet stream that has an 85% selectivity to oxygenates and olefins at 25% cyclohexane feed conversion. Density-Functional Theory (DFT) with B3LYP/6-31+G(d) method for geometry optimizations and thermodynamic analyses was employed using GAUSSIAN08 to predict reaction enthalpies and rate-constant parameters for this system. The major gas-phase reaction channels (29 species, 46 irreversible reactions) were probed by locating stable reactants, products, and transition-state intermediates; and one-dimensional simulations were carried out with CHEMKIN's PLUG program. These calculations gave qualitatively correct trends with cyclohexane/oxygen ratios and dilution. Related work focused on combining the gas-phase kinetics with surface chemistry and two-dimensional fluid dynamics in FLUENT to properly simulate the quenching and surface generated radicals associated with the system.

These researchers also developed surface mechanisms for the partial oxidation of methane over Rh-coated foam monoliths. FLUENT was used in combination with user-

defined subroutines that enable surface/gas-phase chemistry coupling to simulate two-dimensional flow in a tubular catalytic wall reactor. This work focused on the further development of these surface mechanisms to explain the experimentally observed water-gas shift and steam reforming reactions associated with steam addition to this partial oxidation system. FLUENT was used in combination with this refined mechanism to simulate and capture the complex interaction between heat transfer, mass transfer, surface chemistry, and gas-phase chemistry.

Further research was performed in density-functional-theory modeling of cyclohexane partial oxidation in millisecond single-gauze reactors. Cyclohexane oxidation over a Pt-10% Rh single-gauze catalyst can produce ~85% selectivity to oxygenates and olefins at 25% cyclohexane conversion and 100% oxygen conversion, with cyclohexene and 5-hexenal as the dominant products and cyclohexanone a minor product.

Understanding the favored reaction pathways suggests ways to adjust reactor operation for desired product distributions. Detailed numerical simulations of the surface-assisted gas-phase process allowed the investigation of experiments, which are often costly or potentially dangerous to carry out. ■

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Physics of Fluids in Processing Technologies

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

This research formed a part of two 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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Electronic, Structural, and Thermodynamical Properties of Materials

This group's research dealt with the development and application of first principles electronic structure methods, emphasizing the study of solids at high pressures and temperatures. It is very difficult to create high pressure and temperature conditions in controlled laboratory experiments; however, reliable and predictive simulations are possible using first principles constant pressure molecular dynamics and high performance computing. Simulations of solids at high pressures are of extraordinary importance to earth science, since such simulations predict the structural and elastic properties of earth forming materials. Their knowledge is required to provide a consistent basis for a discussion of the chemistry and physics of the earth's interior.

From a fundamental point of view, high-pressure studies can extend scientific understanding of atomic bonding. Examples of other problems of interest in the Wentzcovitch group included pressure-induced solid-state amorphization, zeolite aluminosilicates, alumina and ruby, and, more recently, magnetic oxides and first principles phonon thermodynamics. ■

Research Group and Collaborator

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George Barany, Principal Investigator

Design and Characterization of Biomolecules: From Protein Core Modules to Cyclic Peptic Nucleic Acid

These researchers studied the engineering of stable, folded, and functional biomolecules, and were particularly interested in the design, synthesis, and characterization of protein core modules and cyclic peptic nucleic acid (PNA).

In globular proteins, core motifs can be identified and their elements combined in suitable peptides to construct native-like modules. The designed peptides consist of core elements from bovine pancreatic trypsin inhibitor (BPTI) and/or B1 immuno-globulin binding domain (GB1) linked by natural or designed sequences, and they contain a strategically placed crosslink 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 for generating nanotubular structures. Such nanotubular reagents can be useful as new catalysts, wire conductors, or drug transport systems. Cyclic PNAs were designed by means of molecular modeling studies that assess the viability of cyclization, as well as the molecular recognition mechanism between cyclic units.

Design and characterization studies in this field are computationally intensive, thus requiring the resources of the Supercomputing Institute. Once the designed molecules are synthesized, they are the subjects of nuclear magnetic resonance (NMR) spectroscopic studies, from which structural features can be calculated. ■

Research Group and Collaborator

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David A. Blank, Principal Investigator

Excited State Intramolecular Proton Transfer Studies of 2-(2-Pyridyl)pyrrole in Solution

This group performed computational investigations of the excited state intramolecular proton transfer in 2-(2-pyridyl)pyrrole in solution. This molecule offers a model system where the geometry for the proton transfer is restricted compared with previous studies of hydrogen bonded dimers. The group employed both *ab initio* and semi-empirical models for the solute and the sm5.42 implicit solvation model to examine the ground and excited states of both in 2-(2-pyridyl)pyrrole and the proton transfer state. They calculated absorption and fluorescence energies using the time-scale separation method developed by Truhlar and coworkers, where the vertical transition energy is obtained by allowing equilibration of only the electronic degrees of freedom in the final state. For example, the absorption maximum will reflect the energy difference between a fully-equilibrated ground state and the excited state calculated with the ground state reaction field where the electronic degrees of freedom have equilibrated in the excited state but the nuclear degrees of freedom remain frozen at the ground state configuration. Fluorescence was calculated from an equilibrated excited state and an electronically equilibrated ground state with a reaction field that reflected the excited state nuclear configuration. These computations will be used in conjunction with spectroscopic experiments to generate a complete picture of this model proton transfer system. ■

Research Group

Sarah Schmidtke, Graduate Student Researcher

Christopher J. Cramer, Fellow

Computational Chemistry

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

- Molecular modeling of transfer ribonucleic acid (tRNA)
- Predicting the dynamical properties of 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

In the first of these they addressed the atomic mutagenesis of tRNA tetraloop analogs. These can be used to better understand the properties of charging RNA with appropriate amino acid. Mutagenesis of a tRNA_{Ala} tetraloop analog structure (solved by nuclear magnetic resonance [NMR], Varani) to C1:G70 does not charge the RNA with alanine. The dynamic behavior of the wild type and the mutant in simulations were compared to better understand their different biological activity. These simulations included the full environment (water, counterions, etc.), taking advantage of recently developed simulation technology (parallel simulation code, Particle Mesh Ewald accounting for long-range electrostatics, etc.).

The group developed a number of new studies in this research period. Among them was a method of quantum chemical characterization of cycloaddition reactions between 1,3-butadiene and oxyallyl cations of varying electrophilicity. Hydroxyallyl cation and lithium and sodium oxyallyl cations were predicted to react with 1,3-butadiene both in a stepwise fashion and via concerted [4 + 3] cycloaddition with so-called extended stereochemistry. With hydroxyallyl cation, the stepwise process is pre-

ferred and subsequent second bond closures generate products equivalent to those that would arise from concerted [4 + 3] or [3 + 2] cycloadditions. For lithium and sodium oxyallyl cations, concerted, asynchronous processes were predicted to be preferred over stepwise processes, with [3 + 2] cycloaddition to generate a 3*H*-dihydrofuran followed by Claisen rearrangement of that intermediate being the lowest energy pathway for formation of a seven-membered ring. In the case of uncharged 2-oxyallyl, only transition state structures for concerted cycloadditions appeared to exist. The researchers inferred that for [4 + 3] cycloadditions, concerted pathways are preferred over stepwise pathways provided that the separation between the electrophilicity of the allyl component and the electrofugacity of the 4p component is not too large. The Hammond postulate was shown to rationalize variations in free energies of activation for different processes as a function of allyl electrophilicity. The researchers also studied the factors influencing the stereochemical outcome of different cycloadditions.

A further area of study by these researchers concerned perspective sugar anomerism. This work presented the first conformational analysis of the anomeric effect within the context of molecular orbital theory, discussed the utility of Fourier decomposition of a torsional coordinate as a method for analyzing disparate electronic influences on that coordinate, and helped settle debate on the nature of anomeric stabilization.

In another study, the researchers demonstrated the feasibility of computational electrochemistry, specifically the calculation of the aqueous one-electron oxidation potentials of substituted anilines. Here, the emphasis was on semiempirical molecular orbital theory and density functional theory as used to compute one-electron oxidation potentials for aniline and a set of 21 mono- and di-substituted anilines in aqueous

Christopher J. Cramer, Fellow

solution. Linear relationships between theoretical predictions and experiment were constructed, providing mean unsigned errors as low as 0.02 V over a training set of 13 anilines; the error rises to 0.09 V over a test set of eight additional anilines. A good correlation was also found between oxidation potential and a simple computed property, namely the energy of the highest occupied molecular orbital for neutral anilines in aqueous solution. For the particular case of the substituted anilines, a strong correlation between oxidation potential and pK_a was found, in conjunction with a still stronger correlation between oxidation potential and physical organic descriptors for aromatic substituents, albeit over a reduced data set.

Another project involved the prediction of soil sorption coefficients using a universal solvation model. Using a database of 440 molecules, the researchers developed a set of effective solvent descriptors that characterize the organic carbon component of soil and thereby allow quantum mechanical SM5 universal solvation models to be applied to partitioning of solutes between soil and air. Combining this set of effective solvent descriptors with solute atomic surface tension parameters already developed for water/air and organic solvent/air partitioning allows one to predict the partitioning of any solutes composed of H, C, N, O, F, P, S, Cl, Br, and I between soil and water. The researchers also presented linear correlations of soil/water partitioning with 1-octanol/water partition coefficients using the same database. The quantum mechanical calculations have the advantages that they require no experimental input and should be robust for a wide range of solute functionality. The quantitative effective solvent descriptors can be used for a better understanding (than with previously available models) of the sources of different partitioning phenomena in cases where the results exhibit significant fragment interactions. From this work, the

researchers anticipated that the model would be useful for understanding the partitioning of organic chemicals in the environment between water and soil or, more generally, between water and soil or sediments (geosorbents). A measure of partitioning between soil organic matter and water, normalized to organic carbon content, was taken for analysis. The availability of measured values of K_{OC} for a large number of organic compounds has prompted many efforts to develop predictive models for this quantity. Such models are useful in providing estimates that may avoid the need for experimental measurements or assist in optimizing the methodology employed for those measurements as well as for environmental modeling. Linear correlations between K_{OC} and other measured solute properties (and nonlinear correlations between K_{OC} and $P_{O/W}$ or other solute properties) were also developed. ■

Research Group and Collaborators

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Design of Semisynthetic Enzymes Based on Fatty Acid Binding Proteins

The objective of this work was to develop enantioselective catalysts 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 deoxyriibonucleic 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 were 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 catalysts to include C–C bond formation

Computer modeling was central to the accomplishment of the aims of this project. ■



This stereo picture of hslFABP-FL60 (flavin conjugate) was generated by insightii/discover based on one of the nuclear magnetic resonance (NMR) structures. The ball-and-stick structure illustrates the flavin moiety conjugated to the Cys₆₀ residue of helixless IFABP.

Research Group

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Computer Simulations of Chemical and Biochemical Systems in Solution

In this group, a multi-faceted computational project is directed to the study of:

- The dynamics and mechanism of enzyme-catalyzed reactions
- The structure and interactions of membrane proteins
- Solvent effects on chemical reactions and interactions in condensed phases

The approach adopted by the group was based on statistical mechanical Monte Carlo and molecular dynamics simulations, making use of a combined quantum mechanical and molecular mechanical (QM/MM) potential.

The first project area involves research into a variety of enzymatic reactions, making use of combined QM/MM methods in molecular dynamics simulations. The group has completed the hydride transfer reaction catalyzed by alcohol dehydrogenase, zyllose, and methylamine dehydrogenase, as well as the dihydrofolate reductase reaction path. On-going research involves the human protein tyrosine phosphatase B (PTP1B), squalene cyclases (involved in cholesterol biosynthesis), decarboxylation reactions catalyzed by orotidine phosphate decarboxylase and pyruvate decarboxylase, and hydride transfer reactions catalyzed by dihydrofolate reductase and acyl-CoA dehydrogenase. These studies 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 area 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 project's computational details are similar to those of a previous study done by this group involving the protein bacteriorhodopsin. The group is 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 the sensory protein, photoactive yellow protein.

The third project area focuses on the development of novel computational techniques in combined QM/MM calculations and applications to modeling the hydrolysis of model compounds for glycosyl derivatives and solvent effects on hydride transfer reactions as models for enzymatic processes. The study of solvents is important in the understanding of the reaction mechanism of organic reactions. The group modeled organic reactions having large solvent effects. The reactions also served as model systems for enzymatic processes. The two reactions the group studied were the hydrolysis of α -methoxy tetrahydropyranoside and the hydrolysis of methyl phosphate. The first reaction is a model compound for the reaction of glycosyl derivatives; the second is a model for kinase and phosphatase catalysis. These simulations used QM/MM Monte Carlo simulations, typically involving $5\text{--}10 \times 10^7$ configurations. ■

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Design of Peptidomimetics as Anti-HIV and Antiangiogenic Antitumor Agents; Computation of Proton and Carbon NMR Chemical Shifts

Molecular modeling is a powerful tool for guiding the design of new targets for organic synthesis. Identification of novel biologically active agents is one valuable application.

This research group engaged in designing non-peptidic analogs based on known, active peptidic lead compounds. Representative examples of projects where such approaches benefit this research are:

- The design of a new class of enzyme inhibitors as potential anti-HIV (human immunodeficiency virus) agents. These were based upon structural information available from crystallographic studies of complexes between various peptidic agents (cyclosporin A and p55gag fragments) and human cyclophilin A. It is clear that the latter, host-cell protein must be recruited into new HIV virions to render the latter infective.
- The design of new antiangiogenic antitumor agents. These were based upon knowledge of a requirement for certain side chain substituent nature and relative orientation in known antiangiogenic polypeptidic agents.

Design of structures built on scaffolds displaying these residues in similar fashion were guided by modeling studies.

A new project initiated by this team uses nuclear magnetic resonance (NMR) spectroscopy to determine the three-dimensional structure (i.e., stereostructure, which encompasses 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 unambiguously determining complete stereochemical structures are of considerable value. The researchers have begun to develop

new methodologies that involve the comparison of computed with experimental spectroscopic parameters. The two principal types of information that are at the very core of nearly all NMR spectroscopic analyses are *chemical shifts* (δ) and *coupling constants* (J). In principle, these values can be computed for an entire family of possible stereoisomers and then compared with the experimental values to allow for deduction and assignment of the correct structure. The hypothesis is that comparison of computer 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

Ab initio molecular orbital and density functional calculations were carried out on a variety of organic systems during this research period. Particular attention was paid to 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.

Specific work within this overall research focus produced a number of results. For example, the researchers considered the impact of fusing a strained ring onto benzene. The gas-phase acidities of the two aromatic sites in benzocyclobutene were measured in a Fourier transform mass spectrometer using a kinetic technique (i.e., the DePuy method). Fusion of a cyclobutane ring onto benzene was found to have a slight acidifying effect on the α -position (3.2 ± 1.7 kcal mol⁻¹) and little, if any, influence on the β -site (0.8 ± 1.9 kcal mol⁻¹). Energetic data ($\Delta H^\circ_{\text{acid}} = 386.2 \pm 3.0$ kcal mol⁻¹, $EA = 0.84 \pm 0.11$ eV, and C-H BDE = 92 ± 4 kcal mol⁻¹) for the benzylic position were obtained via the bracketing technique and application of a thermodynamic cycle. Differences in the reactivities of the three conjugate bases also were explored. *Ab initio* and density functional theory calculations were carried out to provide geometries, energies, and insights into the carbanions' electronic structures.

Also in this period, benzocyclobutadienyl diazine was synthesized and reacted with hydroxide ion in a Fourier transform mass spectrometer to produce the conjugate base of benzocyclobutadiene (1a). Authentication of the ion structure was carried out by a derivatization experiment (i.e., 1a was converted to benzocyclobutenone enolate, which has previously been studied), and its reactivity was

explored. Thermochemical data for benzocyclobutadiene were obtained ($\Delta H^\circ_{\text{acid}}(1) = 386 \pm 3$ kcal mol⁻¹, $EA(1r) = 1.8 \pm 0.1$ eV, and C-H BDE (1) = 114 ± 4 kcal mol⁻¹), compared to MP2 and B3LYP calculations, and contrasted with a series of model compounds. Cyclobutadienyl radical appears to be quite different from benzocyclobutadienyl radical (1r) and worth further exploration.

In another experiment, dodecahedryl anion (1a) was generated in a Fourier transform mass spectrometer by deprotonation of dodecahedrane (1). Examination of the acid and base behavior of 1 and 1a, respectively, enabled the acidity of 1 to be determined ($\Delta H^\circ_{\text{acid}} = 402 \pm 2$ kcal/mol). Good agreement is found with the 298 K computed MP2/6-31 + G(d)//HF/6-31 + G(d) value of 405.1 kcal/mol. In a similar manner, the electron affinity of dodecahedryl radical was measured ($EA = 4 \pm 2$ kcal/mol). These results were combined in a thermodynamic cycle to afford the C-H bond dissociation energy of dodecahedrane (BDE = 92 ± 3 kcal/mol), which is reasonably well reproduced (96.7 kcal/mol) at the MP2/HF level but leads to the suggestion that the reported heat of hydrogenation of dodecahedrene is in error. The DePuy kinetic method for measuring the acidity of 1 also was explored. It was found that this approach works well with triphenylsilyldodecahedrane but gives poor results with triethylsilyldodecahedrane. This latter failure is attributed to steric effects, and provides a rationale for several problem cases and a means to overcome these difficulties.

Furthermore, benzocyclobutadiene radical anion (5) was synthesized by the researchers in the gas phase by three independent approaches: collision-induced dissociation (CID) of 1,2-benzocyclobutenedicarboxylate, reaction of 2-trimethylsilyl-1-benzocyclobutenyl anion with neopentyl nitrite followed by CID of the resulting β -nitroso carbanion intermediate, and reac-

tion of the same β -silyl carbanion with molecular fluorine. The proton affinity and electron binding energy of **5** were measured (0.32 ± 0.05 eV and 368 ± 2 kcal mol⁻¹ respectively) and combined in a thermodynamic cycle to obtain the heat of hydrogenation (49 ± 4 kcal mol⁻¹) and the heat of formation (97 ± 4 kcal mol⁻¹) of benzocyclobutadiene (**1**). These results were compared to model compounds as well as MP2 and B3LYP calculations in order to assess the antiaromatic destabilization energy of **1**. Based on this data, a predicted heat of formation of cyclobutadiene (102 kcal mol⁻¹) was obtained. This work demonstrated the utility of dicarboxylates as radical anion precursors and the electron as a protecting group.

In addition to these projects, the research group generated dicarboxylates by electrospray ionization mass spectrometry and found that they lose carbon dioxide and an electron upon collision-induced dissociation to afford distonic ions. These radical anions can also be synthesized via laser desorption, chemical ionization, and electron ionization of dibenzyl esters. Subsequent fragmentation of the remaining CO₂ affords new radical anions corresponding to neutral reactive intermediates. By measuring the proton affinities and electron binding energies of these species, quantitative energetic information on carbenes, biradicals, and other transient molecules can be obtained. This approach was demonstrated by measuring the heats of formation of 2,3- and 2,6-dehydronaphthalene; ancillary thermochemical data also were derived, and the results were then compared to either *o*- or *p*-benzyne.

Yet another project sought to probe electrostatic effects using the formation and characterization of zwitterionic ions and their “neutral” counterparts in the gas phase. A dipolar ion and its non-zwitterionic counterpart were generated and characterized in the gas phase. A single charge site was found to be sufficient to

lower the energy of a zwitterion well below its neutral counterpart. Charge separation in a dipolar anion enables hydrogen–deuterium exchange to take place with acids over an extraordinarily large range. These results provide a basis for studying electrostatic effects and understanding mass spectroscopic processes involving large biological molecules. ■

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Computational Studies of Partially Bound and Hydrogen Bound Complexes

Supercomputing resources were used by these researchers for the purpose of carrying out high-level quantum chemical calculations on partially bonded molecules. The results of these studies served to enhance the group's ongoing experimental studies, both by providing detailed information concerning bond energies and medium effects, and also by allowing a more accurate prediction of molecular structure. ■

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Importance of Discriminator Base Stacking Interactions: Molecular Dynamic Analysis of A73 Microhelix^{Ala} and Microhelix^{His} Variants

Transfer of alanine from *Escherichia coli* alanyl-transfer ribonucleic acid (tRNA) synthetase (AlaRS) to RNA minihelices that mimic the amino acid acceptor stem of tRNA^{Ala} was shown, by analysis of variant minihelix aminoacylation activities, to involve a transition state sensitive to changes in the “discriminator” base at position 73. Solution nuclear magnetic resonance (NMR) indicated that this single-stranded nucleotide is predominantly stacked onto G1 of the first base pair of the alanine acceptor stem helix. These researchers observed the activity of a new variant with the adenine at position 73 substituted by its non-polar isostere 4-methylindole (M). Despite lacking N7, this analog is well tolerated by AlaRS. Molecular dynamics (MD) simulations show that the M substitution improves position 73 base stacking over G1, as measured by a stacking lifetime analysis. Additional MD simulations of wild-type microhelix^{Ala} and six variants reveal a positive correlation between N73 base stacking propensity over G1 and aminoacylation activity. For the two DN7 variants simulated, the researchers found that the propensity to stack over G1 was similar to the analogous variants that contain N7, leading to the conclusion that the decrease in aminoacylation efficiency observed upon deletion of N7 is likely due to loss of a direct stabilizing interaction with the synthetase.

These researchers also performed work in conformational analysis of histidine tRNA acceptor stem models. Histidine tRNA is unique in that its acceptor stem has only a single strand of three nucleotides rather than the four nucleotides common to most tRNAs. This is due to the fact that the discriminator base (C73) is paired with a G-1. Conformations of several tRNA acceptor stems have previously been studied to determine the role of the tRNA conformation in recognition by the cog-

nate synthetase. However, the effect of a C in the discriminator position has never been studied and the conformation of the unique tRNA^{His} acceptor stem sequence is unknown. The goal of this project is to determine the conformation of the acceptor stem model microhelix^{His}, both wild-type (with a G at position -1) and without the G-1. To date, the RNA samples have been prepared and solution NMR experiments have been completed. Constraint files were generated to model the acceptor stems using the program amber. Molecular dynamics simulations were carried out with the NMR generated distance constraints, solvated with explicit water. ■

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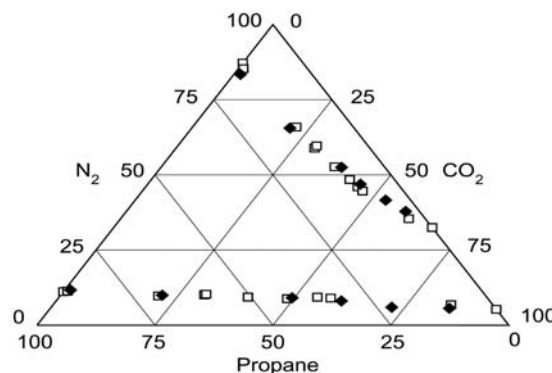
J. Ilja Siepmann, Fellow

Simulating Complex Chemical Systems

The efforts of this research group were driven by the desire to learn about complex chemical systems on the microscopic level and to predict accurate thermodynamic data for these systems. The research performed by the group helped in the understanding of how molecular architecture and composition influence structure, phase behavior, and function of the resulting complex systems. The main research tool of this group is particle-based computer simulation, and the in-house development of efficient simulation algorithms and transferable force fields allows this group to address complex chemical systems, which are not amenable to conventional simulation approaches and for which experimental data are not readily accessible.

Algorithm Development—This group proceeded on the development of three novel Monte Carlo algorithms that target the efficient sampling polymer systems, strongly associating fluids, and polarizable force fields. First, the self-adapting fixed-endpoint configurational-bias Monte Carlo (SAFE-CBMC) method enabled this group to carry out conformational changes for interior segments of chain molecules with strong intramolecular interactions. This CBMC method allowed for the efficient simulation of cyclic alkanes (or other ring structures), and was also instrumental for the sampling of polymeric molecules (with more than, for example, 20 repeat units) where conventional CBMC would allow only for conformational changes close to the chain ends.

Second, the aggregation volume bias Monte Carlo (AVBMC) method greatly increased the sampling efficiency for strongly associating fluids. These fluids exhibit large deviations from the ideal-gas or ideal-solution behavior and pose a special challenge for molecular simulation because aggregate formation leads to traps in phase space, i.e., configurations that have a very large Boltzmann weight associated with the large favorable energies of cluster forma-



Ternary phase diagram for CO₂/N₂/propane at 270 K and 60 bar. Squares and diamonds depict the experimental data (Yucelen and Kidnay, *J. Chem. Eng. Data*, **44**, 926 [1999]) and the simulation data for the TraPPE-EH force field, respectively.

tion. However, these “bonded” configurations represent only a small fraction of the total phase space compared to the large amount of non-bonded configurations.

Third, the adiabatic nuclear and electronic sampling Monte Carlo (ANES-MC) method allows simulations using polarizable force fields. In close analogy to the revolutionary Car-Parrinello molecular dynamics method, the ANES-MC algorithm for polarizable force fields treats the molecular charge distributions as additional variables. While the Car-Parrinello molecular dynamics method is able to exploit an extended Lagrangian formalism and benefits from the faster motion of the electronic degrees of freedom, the ANES-MC algorithm allows for the sampling of nuclear and electronic degrees of freedom with different temperatures by sandwiching a sequence of electronic moves in between the nuclear trial displacement.

Force Field Development—The success of molecular simulation in predicting thermophysical properties depends on the availability of accurate force fields. This group made progress in the development of a multi-level force field, called “transferable potentials for

phase equilibria" (TraPPE). The first-level force field, TraPPE-UA (united atom), employs the united-atom representation for alkyl segments and simple Lennard-Jones and Coulombic terms. In the second level, TraPPE-EH (explicit hydrogen), all atoms including alkyl group hydrogens and some lone-pair electron and bond-center sites are treated explicitly. In the third-level, TraPPE-pol (polarizable), both the van der Waals and electrostatic interactions can respond to changes in the environment. Whereas the first level is designed for simplicity and computational efficiency with good accuracy, the second level is aimed at improved accuracy for mixtures of non-polar or apolar non-hydrogen-bonding compounds. The third level is directed solely at the highest possible level of accuracy and transferability.

Extensions were made to the TraPPE force fields as follows. TraPPE-UA models for alkenes, aromatics, alcohols, ethers, ketones, and aldehydes; TraPPE-EH model for dinitrogen, carbon dioxide, and linear alkanes (see figure); and TraPPE-pol models for water.

Applications—This group investigated the binary mixture of *n*-heptane and supercritical ethane. Pressure-composition and temperature-composition phase diagrams were computed using four different molecular models of increasing complexity. In the supercritical phase, preferential solvation of heptane by ethane is not observed. Analysis of the contributions of the liquid and the supercritical phase to the decrease of the Gibbs free energy of transfer of heptane with increasing pressure suggest that the enhanced solubility of heptane in high-pressure supercritical ethane can be attributed to two causes of roughly equal importance: "pulling" of heptane into the supercritical phase by an increased density of ethane that acts as a non-specific solvent, and "pushing" heptane out of the liquid phase by an increased concentration of ethane.

Octanol-water partition coefficients are extraordinarily successful for correlating and predicting numerous processes of pharmacological and environmental importance. However, the structural details of the octanol phase, and the reason why this phase can mimic the complexities of many different environments ranging from biomembranes to soil, are controversial. This group investigated the partitioning of normal alkane and primary alcohol solutes between water and (dry or wet) 1-octanol phases using the OPLS-UA and TraPPE-UA force fields. It was found that the TraPPE-UA model yields superior results (e.g., a dramatic increase in the mutual solubility of water in octanol). Comparison of the partitioning between a helium vapor phase and dry and wet 1-octanol established that water saturation affects mostly the partitioning of polar solutes, while differences for alkane partitioning were found to be negligible. Analysis of the microscopic-level structure of the wet 1-octanol phase shows preferential partitioning of short alcohols (methanol and ethanol) into the water-rich regions of the microheterogeneous solvent mixture, whereas 1-butanol solutes are found preferentially at the boundary of hydrogen-bonded clusters. These simulations demonstrate that a diverse spectrum of hydrogen-bonded aggregates exists in neat and wet 1-octanol, and that water saturation substantially alters the 1-octanol environment. The simulation results are able to reconcile the conflicting views of the 1-octanol structure inferred from thermodynamic arguments, spectroscopic measurements, and diffraction experiments.

Configurational-bias Monte Carlo simulations in the grand canonical ensemble with histogram reweighting were used to determine the vapor-liquid coexistence curves and critical parameters for a few linear and branched alkanes physisorbed on a flat gold substrate. Examination of the critical ordering operator distributions confirms that these systems exhib-

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it critical behavior consistent with the two-dimensional Ising universality class. It was shown that a principle of corresponding states does not hold true between bulk fluids and adsorbed monolayers. The ratio of the two-dimensional to three-dimensional critical temperatures was found to decrease with chain length for *n*-alkanes (from about 0.38 for methane to 0.30 for *n*-hexane). In contrast to typical bulk fluid behavior, the branched isomers were found to have higher critical temperatures than their linear counterparts.

Gas-liquid and reversed-phase liquid chromatography are the principal methods for the analysis and separation of organic and pharmaceutical molecules. Due to the complexity of chromatographic systems and the lack of microscopic-level information, however, many fundamental questions on the retention mechanisms remain unanswered. Accurate predictions of retention times, retention indices, and partition constants are a long sought-after goal for theoretical studies in chromatography. This group studied the retention of linear and branched alkanes and of alkylbenzenes in helium-squalane gas-liquid chromatography. Configurational-bias Monte Carlo (CBMC) simulations in the Gibbs ensemble using the TraPPE-UA force field were carried out to obtain a microscopic picture of the partitioning of 10 alkane isomers and of benzene, toluene, *o*-, *m*-, and *p*-xylene between a helium vapor phase and a squalane liquid phase, a prototypical gas-liquid chromatography system. The alkane solutes include some topological isomers that differ only in the arrangement of their building blocks (e.g., 2,5-dimethylhexane and 3,4-dimethylhexane or the xylene isomers), for which the prediction of the retention order is particularly difficult. The Kovats retention indices, a measure of the relative retention times, were calculated directly from the partition constants and are in good agreement with experimental values. The calculated Gibbs free

energies of transfer for the normal alkanes were shown to conform to Martin's equation, which is the basis of linear free energy relationships used in many process modeling packages. Analysis of radial distribution functions and the corresponding energy integrals did not yield evidence for specific retention structures and showed that the internal energy of solvation is not the main driving force for the separation of topological isomers. This work was highlighted in "Analytical Currents" (*Analytical Chemistry*, p. 185 A [March 1, 2000]) and described in terms of climbing "the Mt. Everest of separation science." ■

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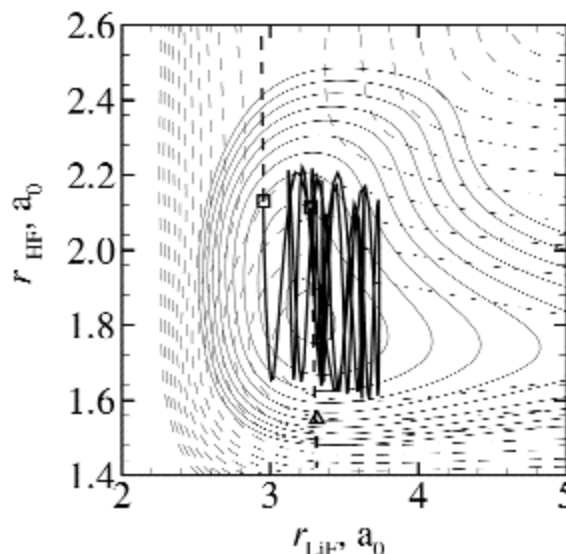
Computational Chemical Dynamics

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 on structure and dynamics. A combination of quantum mechanical, quantum statistical, semiclassical, and classical mechanical methods is used to perform the calculations.

In one project, the group developed a set of multi-coefficient correlation methods (MCCMs) that combine self-consistent-field and correlated electronic structure calculations to extrapolate to infinite order of electron correlation and a complete one-electron basis set. These are optimized against a database of atomization energies, ionization potentials, electron affinities, and barrier heights. This leads to a suite of four MCCMs (called MCG3/3, MC-QCISD/3, MCCO/3, and SAC/3) that have excellent performance-to-cost ratios with a broad range of cost-per-size scalings such that they are applicable to both large and small systems. The new methods are also very efficient for computing geometries of open-shell transition states.

Another electronic structure method developed by these researchers is a new hybrid Hartree-Fock-density functional (HF-DF) model, called the modified Perdew-Wang 1-parameter model for kinetics (MPW1K). This model was optimized against a database of 20 forward barrier heights, 20 reverse barrier heights, and 20 energies of reaction. The results were then compared to other hybrid HF-DFT methods with the 6-3+G(d,p) basis. The new method reduces the mean unsigned error in reaction barrier heights by a factor of 2.4 over mPW1PW91 and by a factor of 3 over B3LYP.

The group also made progress in developing new dynamics methods for photochemical reactions. First, they studied classes of semiclassical (mixed quantum mechanical/classical)



A surface-hopping trajectory used by Jasper and Truhlar to model the decay of the LiFH exciplex to LiF + H is illustrated as a thick line, on a background of potential energy contours shown as thin lines. The trajectory is shown as a thick solid line when it occupies the excited electronic state (solid contours) and as a thick dashed line when it occurs the ground electronic state (dashed contours). The trajectory starts in the excited-state well, goes through several HF vibrations, hops to the ground state (square), stretches along the HF distance, hops non-locally (i.e., tunnels) to the excited state (triangle), goes through several more excited-state HF vibrations, hops again to the ground state (square), and finally goes on to form H + LiF. The ordinate is the H-to-F distance in bohrs ($1 a_0 = 1 \text{ bohr} = 0.53 \text{ angstroms}$), and the abscissa is the Li-to-F distance in bohrs.

methods for investigating multi-electronic-state dynamics: the trajectory surface hopping (TSH) method and the time-dependent self-consistent field (TDSCF) method. The recent development in their group of the capability to calculate accurate quantum mechanical reaction probabilities for a variety of realistic three-body, two-state potential energy matrices allowed an assessment of the validity of semi-

Donald G. Truhlar, Fellow

classical multi-surface dynamics methods that are applicable to larger systems. These studies indicate that Tully's fewest-switches algorithm augmented by a new time uncertainty algorithm for tunneling is the best available TSH method and that the Ehrenfest method is the best previously available TDSCF method. The fewest-switches surface hopping method has relatively small errors, even when it is not the best method, while the Ehrenfest TDSCF method tends to have larger errors when it is not the best. However, the fewest switches algorithm involves unphysical discontinuities in momenta, and the results may depend on the choice of representation. Furthermore, the new surface hopping algorithm is sometimes frustrated in its attempt to maintain ensemble-average self consistency, although the time-uncertainty tunneling algorithm has greatly reduced this problem. The Ehrenfest method removes all these troublesome aspects but at the cost of producing unphysical mixed states that are responsible for its larger errors in observables.

An improved time-dependent self-consistent-field method for nonadiabatic dynamics was also developed. The method is a variant of the time-dependent self-consistent field method and is called "continuous surface switching." The algorithm combines the best features of the self-consistent-potential trajectory-surface-hopping approach and the Ehrenfest classical-path self-consistent-potential approach without their relative disadvantages. Viewed from the self-consistent perspective, it corresponds to "on-the-fly histogramming" of the Ehrenfest method by a natural decay of mixing; viewed from the surface hopping perspective, it corresponds to replacing discontinuous surface hops by continuous surface switching. Accurate quantum mechanical scattering calculations were carried out for three cases by a linear algebraic variational method, and the accurate values of reactive probabilities, quenching

probabilities, and moments of final vibrational and rotational distributions were compared to the results of continuous surface switching, the trajectory surface hopping method in two representations, the time-dependent self-consistent-field method, and the Miller-Meyer classical electron method to place the results of the semiclassical methods in perspective.

Another example of the work performed by this group was the development of a new potential energy surface for the gas-phase reaction $\text{Cl} + \text{CH}_4 \rightarrow \text{HCl} + \text{CH}_3$. Based on the analytical function of Jordan and Gilbert for the analog reaction $\text{H} + \text{CH}_4 \rightarrow \text{H}_2 + \text{CH}_3$, it was calibrated by using the experimental thermal rate coefficients and kinetic isotope effects. The forward and reverse thermal rate coefficients were calculated using variational transition state theory with semiclassical transmission coefficients over a wide temperature range, 200–2500 K. The researchers found that excitation of C–H stretching modes and Cl–H stretching modes enhances the rate of both the forward and the reverse reactions, and excitation of the lowest-frequency bending mode in the CH_4 reactant also enhances the rate coefficient for the forward reaction. However, the vibrational excitation of the CH_4 umbrella mode (lowest-frequency mode in products) slows the reverse reaction at temperatures below 1000 K, while above 1000 K it also accelerates the reaction.

Another new project involved the development of new techniques for the calculation of quasidiabatic states and quasidiabatic potential energy matrix functions for non-Born-Oppenheimer dynamics calculations. The new methods involve an extension of the concept of configurational uniformity, new methods to define diabatic states, and efficient algorithms for implementing these ideas in existing electronic structure codes so that the new states, potential energy surfaces, and couplings can be

calculated by transforming adiabatic states calculated with those codes.

A considerable portion of this group's effort involves variational transition state theory with multidimensional tunneling (VTST/MT). The algorithm for large-curvature tunneling calculations was improved in two ways, in particular by a better treatment of anharmonicity and by increasing the efficiency through a new interpolation algorithm.

The VTST/MT method has now been tested against quantum mechanical calculations for four-body and six-body systems, and the accuracy has been found to be excellent. The method was then used for direct dynamics calculations on the reaction of H with CH₄. By taking advantage of the high dynamical efficiency of VTST/MT, the calculations could be carried out with very high level methods, including state-of-the-art MCCMs. Both rate constants and kinetic isotope effects were calculated and compared with all available experimental data. Finally, a multi-configuration molecular mechanics method was developed for the automatic fitting of potential energy surfaces for use in such dynamics calculations.

The VTST/MT method can also be applied to study reactions occurring in the condensed phase in water and organic solvents by using continuum solvation models. The group developed a new class IV charge model and has begun using it to develop a new continuum solvation model that will be appropriate for studying nucleophilic substitution reactions.

Another project involved the development of a new set of protocols for calculating enzyme catalyzed reaction rates. The new method is called ensemble-averaged variational transition state theory with multidimensional tunneling (EA-VTST/MT). It has several important features over many currently popular algorithms, in particular:

- Ensemble averaging over conformations of

the substrate and the protein is included by full molecular dynamics sampling

- Vibrations are quantized
- The dynamical bottleneck is found dynamically and separately optimized for different ensemble members
- Multi-dimensional tunneling is included in both the small-curvature and large-curvature approximations

The new theory was applied successfully to enzyme reactions involving both large and small amounts of tunneling and to a hydride transfer reaction in which metal-metal motion is an important part of the reaction coordinate.

Another progress area involves the development of new techniques for simulating the dynamics of Al nanoparticles and their reactions with hydrocarbon fragments.

Finally, considerable progress has been made on the use of Feynman path integrals for calculating absolute free energies of anharmonic molecules, including vibration-rotation coupling.

New work begun by the research team involved key applications of the multi-configuration molecular mechanics algorithm to problems in five key areas: combustion, atmospheric chemistry, environmental chemistry, organic reactions in solution, and enzyme reactions. The team began to develop an extension in which a high-level quantum mechanical calculation is combined with a low-level quantal calculation, whereas in the original algorithm, the high-level quantum mechanical calculation is combined with a classical molecular mechanics calculation. ■

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Structure Determination of Membrane Proteins by NMR

This group studied membrane protein structure, dynamics, and interactions with bioactive compounds using nuclear magnetic resonance (NMR) spectroscopy methods. Membrane proteins constitute 15–30% of the genomic sequences and mediate most of the vital cellular activities, functioning as receptors, transporters in channels, and the like. In spite of its biological importance, membrane protein research is lagging behind studies of soluble proteins. This gap will likely be widened by the structural genomic projects. Indeed, conventional structural biology techniques are hampered by the presence of lipids, which are crucial to maintain membrane proteins' structural and functional integrity. Solution and solid-state NMR methods have emerged as a combined approach to solve the structure of membrane proteins in lipid environments. Using solution NMR methods, it is possible to determine the structure of small and medium-sized membrane proteins in detergent micelles.

Solid-state NMR techniques offer precious information on membrane protein topology and organization in lipid bilayers and promise to be an independent method for structure determination. To obtain the final structures, the NMR data are modeled by using computational methods such as simulated annealing and molecular dynamics calculations. This group is using CNS, XPLOR, and other programs for structural analysis such as PROCHECK-NMR and AQUA. ■

Research Group

Mascioni Alessandro, Graduate Student Researcher

Darrin M. York, Principal Investigator

New Methods for Molecular Simulation and Quantum Mechanical Studies of Biomolecules

This research group designs and applies new computational methods to study biomolecules in aqueous solution.

Their particular focus is on four main areas:

- Molecular simulation
- Combined quantum mechanical/molecular mechanical (QM/MM) methods
- Linear-scaling electronic structure methods
- A new density functional theory-based many-body force field

The methods target one of the most challenging areas of computational biochemistry: the accurate atomic-level modeling of deoxyribonucleic acid (DNA) and ribonucleic acid (RNA) and their interactions with metal ions. Systems of particular interest are the hammerhead ribosome, a small self-cleaving RNA catalyzed by bound Mg^{2+} ions. To study the reaction using accurate hybrid QM/MM methods, the group has proposed a new semi-empirical d-orbital specific reaction parameter Hamiltonian. Moreover, they introduced new quantum indices for macromolecular characterization using linear-scaling electronic structure methods applied to DNA and RNA systems. Finally, the group is performing density-functional calculations of electronic polarizabilities of biological molecules and secondary structural motifs in order to create a benchmark data set for the design of new polarizable force field models. ■

Research Group

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Brent Gregersen, Graduate Student Researcher
Anguang Hu, Supercomputing Institute Research Scholar
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Kevin Range, Graduate Student Researcher
Helen Smagin, Undergraduate Student Researcher
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Zeb Thomas, Staff
Sacha Zlatkova, Staff

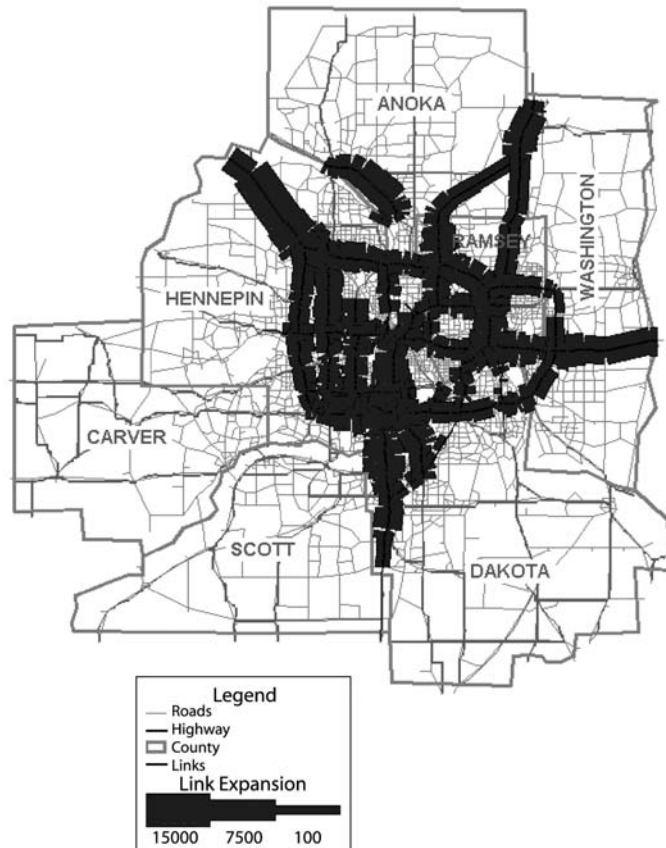
Gary A. Davis, Principal Investigator

Building Our Way Out of Congestion? Network Design for the Twin Cities

An active subject of debate in the Twin Cities of St. Paul and Minneapolis concerns the extent to which new highway construction can accommodate the growth in travel demand expected over the next 20–25 years. These researchers investigated the feasibility of using new highway construction as the sole accommodation to the Twin Cities' projected growth. This was accomplished by solving for a set of expansions of the capacities of freeway segments that, after accounting for the tendency of drivers to divert to faster routes, minimized the land needed for new freeway capacity, while guaranteeing speeds of about 60 mph during the morning and afternoon peak periods. Since the road network model for the Twin Cities contained 1,200 zones and over 20,000 links, this was a very large-scale nonlinear optimization project, but by exploiting the problem's special structure, it was possible to find a numerically efficient solution procedures. Overall, "Building Our Way Out of Congestion" would require about 1,150 additional lane-miles of limited-access roadway. This represents an expansion of about 70% over the current system. ■

Research Group

Katherine Sanderson, Graduate Student Researcher



Year 2020 minimal capacity expansions needed to guarantee essentially uncongested speeds during morning and afternoon peak periods.

Robert J. Dexter, Principal Investigator

Finite-Element Modeling of Steel Structures

During the 1994 Northridge earthquake in California, the connections of steel girders to columns in steel frame buildings fractured unexpectedly. These catastrophic fractures created a strong need to study the details and design provisions of these connections further.

This group's research project focused on understanding the behavior of the stiffeners in the connections, including the behavior of the column continuity plates and the web doubler plates. Analysis was conducted using ABAQUS. These parametric studies were used to compare the experimental results and to aid in providing guidelines for new design recommendations of these steel connections.

Finite element models were created for all test specimens. The results of these analyses and an examination of the design provisions for local web yielding and local flange bending were the basis of the experimental specimen selection.

The principal results clarified the need for and design of transverse stiffeners and doubler plates and to gain additional knowledge to create lower-cost, easier-to-fabricate steel structures.

New research begun by this group is intended to develop guidelines for weld repairs on ships. 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 period of 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 research project is intended to develop guidelines for specific repairs and to determine the restored life as a result of these repairs. The proposed research will include both experimental work as well as a parametric study using

finite element analysis. The analysis will be conducted using ABAQUS. These parametric studies will be used to compare with the experimental results and to aid in providing guidelines for optimal repair recommendations. ■

Research Group and Collaborator

Jerome F. Hajjar, Faculty Collaborator

David St-Peter, Graduate Student Researcher

Clifford Youngberg, Graduate Student Researcher

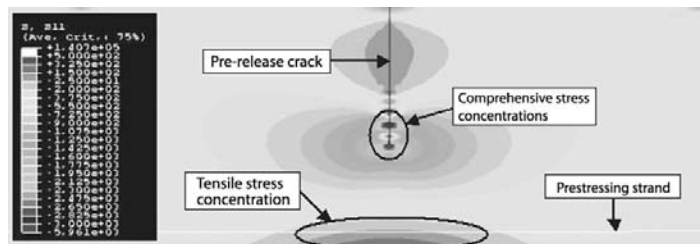
Catherine W. French, Principal Investigator Carol Shield, Co-Principal Investigator

Pre-Release Cracks in Pre-Stressed Girders; Finite-Element Analysis of Integral Abutment Bridges

The objective of this project was to investigate the effect of vertical pre-release cracks on the behavior of pre-stressed bridge girders. As high-strength concrete becomes more popular, heavily reinforced sections with longer span lengths are being used in pre-stressed 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 pre-stressing 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 pre-stressing strands. Following the release of pre-stressing strands, the cracks may close completely due to the effects of pre-stressing 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. A compatibility theory was developed to explain this behavior.

The team has made significant progress towards discovering the effect of pre-release cracks on pre-stressed concrete bridge girders. Analyses done using ABAQUS showed the effects that pre-release cracks have on local girder stresses, flexural cracking load and girder camber.

The current phase of the study includes the experimental validation of the previous analytical study results. ABAQUS was used to optimize the design and instrumentation of test specimens. Models replicating two actual girders have been prepared by ABAQUS to compare the results of the analytical study to available experimental data. The ABAQUS results for camber



Effect of pre-release crack closure on girder stresses.

and stress were found to compare well with the test data. The results of the present analytical and experimental studies will be used to develop recommendations for determining pre-release crack width, depth, and spacing that may present a potential concern for strand fatigue.

This research team is also investigating the behavior of integral abutment bridges using the finite-element program ANSYS. For three years, the team has collected field data from an integral abutment bridge to investigate the effects of environment and vehicle loading on the bridge response. The next step is to conduct an analytical study to develop appropriate models to characterize the bridge's behavior. A key component of this study is the soil-structure interaction caused by seasonal temperature changes and the integral effects of the whole bridge. The results of the analytical study will be compared with the experimental study.

The team has made progress in developing a Finite Element Model (FEM) of the whole bridge using Subgrade Reaction Method to model the soil-structure interaction. The FEM uses shell and beam elements to simulate the superstructure of the bridge, and uses nonlinear springs to model the structure-soil interaction. Current work focuses on comparing FEM results with live load test results. Parametric analyses will also be conducted.

The future research plan continues with both field measurements and numerical studies. ■

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

Research Group

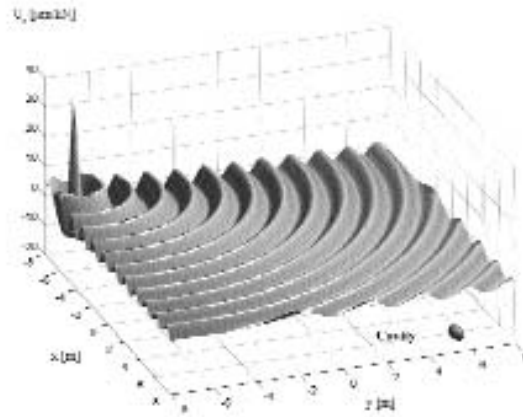
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Tina Wyffels, Graduate Student Researcher

Bojan Guzina, Associate Fellow

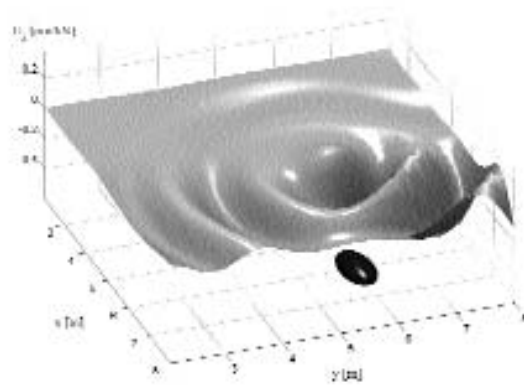
Three-Dimensional Subterranean Imaging via Elastic Waves

The focus of this investigation is the development of a theoretical and computational framework for expedite three-dimensional mapping of underground objects using elastic (i.e. seismic) waves. In contrast to existing computational treatments that require partitioning of an unknown object and its surroundings for simulation purposes, the imaging problem is formulated so that only the outline of an unknown structure is rendered. This approach, which offers formidable computational savings, has its origins in radar and sonar technologies, but has been largely unexplored in the context of seismic imaging. Building on this foundation, this research aims to develop the first three-dimensional, elastic-wave imaging technology that is tractable in the context of a personal computer. Further applications of the methodology may find use in non-destructive material testing and medical diagnosis.

In the first phase of this study, the problem of mapping underground cavities from surface seismic measurements was investigated within the framework of a regularized boundary integral equation (BIE) method. With the ground modeled as a uniform elastic half-space, the inverse analysis of elastic waves scattered by a three-dimensional void were formulated as a task of minimizing the mis-fit between experimental observations and theoretical predictions for an assumed void geometry. For an accurate treatment of the gradient search technique employed to solve the inverse problem, sensitivities of the predictive BIE model with respect to cavity parameters were evaluated semi-analytically using an adjoint problem approach and a continuum kinematics description. Key features of the formulation include the rigorous treatment of the radiation condition for semi-infinite solids and assimilation of the prior information. Numerical results indicate that the featured adjoint problem approach



Vertical ground motion (termed incident field) generated by an axial force vibrating at a frequency of 70 Hz. The scatterer is represented by an ellipsoidal cavity, located two meters beneath the ground surface.



When the incident wave reaches the cavity, part of the energy will be reflected back to the surface. This figure details the latter component of the ground motion (so-called scattered field), which is key information for the imaging problem.

reduces the computational requirements by an order of magnitude relative to conventional finite difference estimates, thus rendering the three-dimensional elastic-wave imaging of solids tractable for engineering applications.

On the forefront of material characterization, this group developed a comprehensive analyti-

Bojan Guzina, Associate Fellow

cal and computational framework for the non-destructive, wave-based testing of lossy (i.e. dissipative) media. By enhancing the treatment of an inverse problem through a fully-coupled viscoelastic analysis of the observed waveforms, the method was designed to provide independent estimates of the *in situ* material stiffness, damping, and density which are not available from conventional seismic interpretations. The presence of noise in experimental observations is accounted for via the use of the maximum likelihood inverse theory. The consistent viscoelastic analysis of waveforms in media with intrinsic dissipation improves the well-posedness of the inverse problem by introducing the internal constraints on the solution which are otherwise absent in traditional (i.e. elastodynamic) seismic analyses. To deal with the significant number of material constants arising in viscoelastic wave interpretation, these researchers also developed a hybrid technique that uncouples the inverse problem via the systematic use of horizontally- and vertically-polarized wave fields.

In parallel with the foregoing developments, this group investigated near-field effects of dynamic interaction between the ground and an impacting annular plate, used worldwide as a seismic source for nondestructive testing of highways. To this end, they developed a mathematical interaction model that demonstrates that the customary uniform-pressure assumption for the contact load between the loading plate and the ground may lead to significant errors in the diagnosis of subsurface pavement conditions. ■

Research Group

Sylvain Nintcheu Fata, Graduate Student Researcher

Andrew Madyarov, Graduate Student Researcher

Miki Hondzo, Principal Investigator

Modeling Nutrient Flux at the Sediment-Water Interface in Aquatic Systems

In spite of increasing computational resources, river, lake, and ocean circulation models cannot resolve all relevant scales of motion; hence, parameterizations for sub-grid scales continue to be necessary. In particular, the kinetics of chemical and biological reactions may be best described at the smallest scales, comparable with (molecular) diffusional length scales. Large-eddy simulation models used to study transport processes in aquatic environments solve the unsteady three-dimensional transport equations for all scales of motion larger than the grid size on the order of 10 m, while the contribution of the sub-grid scales is resolved using a sub-grid scale model.

These researchers were concerned with the study of mass flux at the sediment-water interface in aquatic environments, with specific interest in nutrient cycling. In this research, numerical modeling of phosphorus dynamics in aquatic sediments was used to develop sub-grid scale models that can be used to simulate nutrient dynamics in the water quality models. ■

Research Group

Hector Bravo, Research Associate

Hong Wang, Supercomputing Institute Research Scholar

Raymond 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. This research group is currently involved in a large project investigating the feasibility of promoting biodegradation of chlorinated solvents by using gas-permeable membranes to deliver hydrogen to contaminated aquifers.

As a sub-objective of this research, the group has 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 dechlorination daughter products, plus hydrogen, and methane) and also simulates the growth of three different microbial populations that compete for hydrogen. One of the microbial populations is undesirable because it rapidly consumes hydrogen, but does not degrade chlorinated solvents. However, these researchers have hypothesized that pulsing hydrogen into the groundwater will inhibit the undesirable microbial population while stimulating growth of microbial species capable of degrading 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 soil-free trench in which the H₂-supply membranes are installed.

The domains have different contaminant transport and biotransformation properties and are thus linked by appropriate boundary conditions. A Crank-Nelson finite-differences program has been written in FORTRAN90 to solve the initial value problem.

In order for the group to meet its research objectives, they will perform the following tasks using Supercomputing Institute resources:

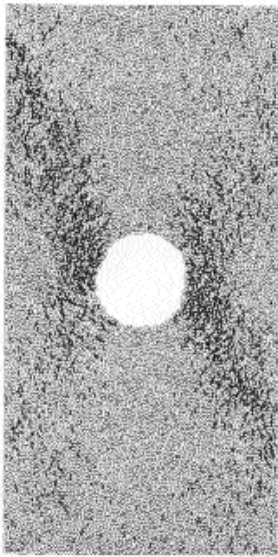
- Perform rigorous finite-differences grid analyses to confirm convergent solutions are attained
- Conduct sensitivity analyses to evaluate the most critical parameters in the model
- Evaluate the system performance under a range of hydrogen pulsing times
- Investigate the potential of using groundwater pumping to increase the hydrogen “zone of influence” ■

Research Group

Lee Clapp, Research Associate

Joseph F. Labuz, Associate Fellow

Characteristic Length of Quasi-Brittle Materials



A micro-mechanical discontinuum program can represent rock by a random assembly of circular particles (grains) bonded together in a dense packing. The resulting distinct model can be regarded as a solid that exhibits deformability through contact stiffness, strength through contact bonds and particle friction, and damage through fracture of bonds. The model produces complex macroscopic behavior such as strain softening and dilation by simulating the micro-mechanisms without resorting to complex constitutive laws. Increases in computing power make it feasible to model entire boundary-value problems with distinct particles such that the constitutive behavior is built into the model; that is, the constitutive response arises from the interaction of a large number of particles, each of which obeys simple contact laws. This approach holds promise for classes of problems where microcracking and localization must be dealt with the design structures.

The objective of this research was to measure the characteristic length of various rocks, which are quasi-brittle materials because they exhibit microcracking. A zone of localized damage prior to failure was mapped with locations of acoustic emission, and space-time clustering analyses helped to define the dimensions. Although the length of this zone may be influenced by loading conditions, the width may be thought of as a material property. In addition, numerical modeling with both finite element and distinct element codes provided a basis for the extension of the experimental results to other materials and conditions. By performing simulations designed to mimic the experimental measure-

ments, the necessary constitutive behavior could be established, and the investigation of boundary value problems could be realized. ■

Collaborator

Ali Fakhimi, Department of Civil Engineering, Tarbiat Modarres University, Tehran, Iran

Joseph F. Labuz, Associate Fellow

Henryk K. Stolarski, Associate Fellow

Identification of Micromechanisms in Failure of Rock-like Materials

A series of non-intrusive testing methods—electronic speckle pattern interferometry (ESPI) and acoustic emission (AE)—were adapted to investigate the failure process of rock and concrete under wedge indentation. To help in identifying the development of micro-cracking, the visualization device in the Supercomputing Institute was used by this research group to determine the deformation process and estimate crack lengths from ESPI experiments. ■

Research Group

Li-Hsien Chen, Graduate Student Researcher

Nathan Iverson, Graduate Student Researcher

Carol Shield, Principal Investigator

Repair of Fatigued Steel Bridge Girders With Carbon Fiber Strips

Several years ago, it was common for steel cover plates to be 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 have been causing fatigue cracks, and some rehabilitation schemes for these cracks have been proposed.

This research focused on carbon fiber reinforced polymer (CFRP) strips bonded to the tension flange as the rehabilitation method for those fatigued tension flanges. In order to use the CFRP strips as the rehabilitation method, it was 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 were conducted to define the development length. The stress distribution in the adhesive of experimental specimens must be similar to that in the rehabilitated girder. Finite element analysis using ABAQUS enabled the researchers to compare those two stress distributions, and to decide which test set-ups can be used. Through preliminary studies, it was found that a large amount of computation time was required to analyze the stress concentration in adhesive, not only due to a singularity at the crack tip but also because of a material non-linearity caused by the high stress concentration. ■

Research Group and Collaborator

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Katsuyoshi Nozaka, Graduate Student Researcher

Henryk K. Stolarski, Associate Fellow

Numerical Analysis of Linear Elasticity Problems With Injectivity Constraints; Investigation of Factors Related to Surface-Initiated Cracks in Flexible Pavements

This team was involved in two areas of research during this period. The first involves solving a problem that occurs with existing linear elasticity solutions for some engineering problems, and that violates one of the basic principles related to deformation of real materials—injectivity. Violation of injectivity leads to a paradoxical situation in which two or more, originally distinct, parts of the deforming body occupy the same physical space after deformation. Although this violation usually occurs in an extremely small region(s), Fosdick and Carfagni have recently shown that this still has very significant influence on the results in the entire domain of analysis.

To rectify this pathological situation, additional local (or differential) injectivity constraints have to be appended to the usual governing equations of the problem. Due to the nonlinear nature of the constraints, a numerical solution procedure is needed, since analytical solutions are not possible, except for very few, simple, one-dimensional problems.

In this work, a finite element model will be developed to solve some of these problems with the injectivity constraints. The constraints will be enforced using Lagrange multipliers. This model will describe a minimization problem with unilateral, non-linear, local constraints, and will lead to a large, highly nonlinear system of equations, which will be solved iteratively.

The second research area concerned surface initiated cracking on roads. Construction and maintenance of pavement structures (roads) require enormous resources and funds. Thus, even small advances in construction practices of roads translate into substantial savings. The researchers are trying to achieve those savings

by a better understanding of mechanisms leading to road deterioration, especially why longitudinal cracking occurs.

In contrast with purely thermal cracking, which typically runs transversely to the road, surface-initiated cracking extends along the road. The phenomenon is not well understood and it is not accounted for in current design procedures. Understanding this relatively new phenomenon would likely lead to improvements extending life of the pavement. Given the costs involved, even small extensions of that life would imply significant monetary savings.

The research is based on the hypothesis (supported by some observations) that tire-road interactions may lead to surface tensile stresses which, compared to the tensile strength of the material involved, is high enough to initiate surface cracking. The team investigated the problem with numerical simulations. The ABAQUS computer program was used to analyze the pavement stress and strain levels in the vicinity of the pavement-tire contact area. The team conducted three-dimensional calculations, changing parameters such as layout of the road layers and their material properties, to determine whether an optimal design exists that minimizes likelihood of cracking. ■

Research Group and Collaborators

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Julie M. Vandenbossche, Graduate Student Researcher

Roger E. A. Arndt, Principal Investigator

Unsteady Sheet/Cloud Cavitation

Cavitation is a significant 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.

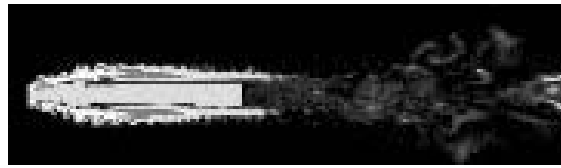
This group's research indicated that sheet/cloud cavitation is a complex and very substantial subset of the overall problem. Focusing on the strongly periodic formation of cloud cavitation that leads to a structured wake consisting of vortical clouds of bubbles, the group found that the phenomenon leads to unsteady lift, which cannot be accurately predicted at this stage. Therefore, the aim was to develop the computational tools to study this problem. Such computational efforts were supplemented by detailed experimental work that is currently underway.

This work included an exploration of the commercial software package *FLUENT 5*'s ability to capture the dynamics of cavitation. The numerical approach used by *FLUENT 5* is part of the Rayleigh-Plesset equation family of cavitation models. This model was implemented along with the Volume of Fluid (VOF) method to track the void fraction in the flow. *FLUENT 5* can calculate the cavitating flow in both three-dimensional and two-dimensional grid systems. The main investigation was performed on a two-dimensional NACA 0015 hydrofoil grid, designed to resemble a test tunnel setup located at St. Anthony Falls Laboratory (SAFL). The study was performed for cavitation numbers ranging from inception to super-cavitation at two different angles of attack. All numerical results were compared quantitatively to corresponding experimental results from the SAFL tunnel. This phase of the study was carried out using the resources made available at the Supercomputing Institute.

A further investigation of the three-dimensional model was performed, using the grid of a



Ventilated test body.



Preliminary computation.

low head Francis hydro-turbine. However, comparison data were not available for this case, a situation that leads to a more qualitative approach than in the two-dimensional case. The numerical investigation of the hydro-turbine was only performed at best efficiency operation. As such, this research showed that the *FLUENT* solver can capture several features of cavitating flows, and can probably be used for industrial purposes.

As an extension of their work on sheet cloud cavitation, this group has broadened their simulations to include ventilated flows and out-gassing due to cavitation. This is important because of the industrial applications of cavitation. The existing model, Arndt et al. (2000), has been modified to include a method for taking into account incondensable gas. Previously, the model only considered condensable vapor. In order to develop and test the model, the group selected ventilated flow as a test case. Ventilation is used in applications of cavity dynamics by injecting air into a region of low pressure, allowing supercavitation to develop at higher values of cavitation number (e.g. free stream pressure). An important question is the amount of ventilated flow required. This question can only be answered if a complete understanding of the physics associated with the bubbly wake trailing such a body is known. ■

Roger E. A. Arndt, Principal Investigator

Research Group and Collaborator

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Quao Qin, Graduate Student Researcher

Travis Schauer, Graduate Student Researcher

Efi Foufoula-Georgiou, Fellow

Space-Time Precipitation Variability and Predictability; Multiscale Recursive Estimation of Precipitation for Applications to Model Variation, Multisensor Estimation, and Data Assimilation

The research efforts of this group were concerned with precipitation space-time variability and predictability.

During this period, the work focused on:

- Quantifying the accuracy of quantitative precipitation forecasts and assessing the limits of predictability of numerical weather prediction (NWP) models as a function of temporal and spatial scale
- Developing a probabilistic framework for interpreting NWP forecasts and assessing their utility for water resources decision-making
- Developing precipitation downscaling methodologies that can be used to disaggregate the large-scale results of regional or global models down to watershed scales for hydrologic applications and also for improving precipitation retrieval from microwave sensors

The first two of these objectives comprised part of a research project: “A Probabilistic Framework for Assessment and Interpretation of Quantitative Precipitation Forecasts from Storm-Scale Models,” funded by the National Science Foundation (NSF). The third objective was part of the research project “Subgrid-Scale Precipitation Variability Over the Mississippi River Basin: A Statistical-Thermodynamic Analysis, Downscaling, and Effects on Water and Energy Partitioning,” funded jointly by the National Oceanic and Atmospheric Administration (NOAA) and the National Aeronautics and Space Administration (NASA), and a research project: “Spatio-Temporal Organization and Space-Time Downscaling of Tropical Rainfall,” funded by NASA.

Precipitation is a highly inhomogeneous process with considerable natural variability at scales ranging from a few meters to several hundreds of kilometers. This process is moni-

tored with a variety of sensors (e.g., rain gauges, radars, and satellites) that provide direct or indirect measurements of precipitation at different resolutions. At the same time, physically-based models at the storm, regional, continental, or global scales are used to predict precipitation, and rely on the observed data for model initialization, model validation, or data assimilation. Due to the tremendous scale-dependent variability of precipitation, merging or comparing observations at different scales or comparing model outputs to observations is not straightforward.

A common approach to Quantitative Precipitation Forecast (QPF) verification is to interpolate the model-predicted areal averages (typically assigned to the center point of the model grid boxes) to the observation sites and to compare observed and predicted point values using statistical scores such as bias and root mean-square error (RMSE). In such an approach, the fact that the interpolated values and their uncertainty depend on the scale (model resolution) of the values from which the interpolation was done is typically ignored. This interpolation error, which comes from scale effects, was construed by these researchers as the “representativeness error” and was quantified as a function of the spatial organization of the storm, the spatial scale of the observations, and the scale (resolution) of the numerical model being verified. This error is a nonzero scale-dependent error even for the case of a perfect model and thus can be seen as independent of model performance. The scale dependency of the representativeness error was shown to have a significant effect on model verification, especially when model performance was judged as a function of grid resolution.

These researchers investigated a new methodology, based on multiscale recursive

Efi Foufoula-Georgiou, Fellow

estimation for optimal merging of precipitation observations at different scales, for data assimilation and for QPF model verification. This technique proved integral to the comparison of observations at different scales while explicitly accounting for their scale-dependent variability and uncertainty. The benefits of the multiscale recursive estimation framework for operational or real-time applications related to multisensor modeling and estimation of precipitation were evaluated.

Further research investigated the accuracy of oceanic tropical precipitation retrieval from microwave sensors during NASA's Tropical Rainfall Measuring Mission (TRMM). The TRMM Microwave Imager (TMI) Goddard Profiling (GPROF) rainfall retrieval algorithm is an inversion type algorithm, which uses numerical cloud models and radiative transfer schemes to simulate the brightness temperatures that the TMI would see, thereby allowing one to relate hydrometeor profiles to brightness temperature. The variability in modeled hydrometeor fields is known to have an important effect on simulated brightness temperatures, and while the TMI instrument sees all the variability down to scales of a few meters, cloud models are typically run at resolutions of 1–3 km, and therefore do not capture the variability at scales less than 5–15 km due to computational mixing. Methods of stochastic downscaling based on wavelets or multiplicative cascades were proposed to reintroduce the missing small-scale variability and reduce the bias in the retrieved precipitation.

On another line of inquiry, these researchers participated in an extensive research effort to characterize and quantify scale invariance in the morphology and evolution of braided rivers. Braided rivers were shown to exhibit anisotropic spatial scaling (self-affinity) in their morphology, implying statistical scale invariance under appropriate rescaling of the axes along and perpendicular to the main direction of

flow. The scaling exponents were found to be similar in rivers of diverse flow regimes, slopes, types of bed material, and braid plain widths, indicating the presence of universal features in the underlying mechanisms responsible for the formation of their spatial structure. In regions where predominant geologic controls or predominant flow paths were present, no spatial scaling was found. Regarding their spatio-temporal evolution, braided rivers were found to exhibit dynamic scaling, implying that a smaller part of a braided river evolves identically to a larger one, provided that space and time are appropriately normalized. Based on these findings and some additional analysis of experimental rivers as they approach equilibrium, the researchers concluded that the mechanism bringing braided rivers to a state where they show spatial and temporal scaling is Self-Organized Criticality, and they have suggested inferences about the physical mechanisms of self-organization. ■

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Ben Tustison, Graduate Student Researcher

Venugopal Vuruputur, Supercomputing Institute Research Scholar

Fernando Porté-Agel, Principal Investigator

Large-Eddy Simulation of Turbulent Transport in the Atmospheric Boundary Layer

The main focus of this research was large-eddy simulation (LES) of turbulent transport in the atmospheric boundary layer. LES consists of numerically solving the unsteady three-dimensional equations that govern the turbulent transport of momentum and scalar quantities such as temperature, water vapor, and pollutants. Until now, LES has not been adequate for studying the atmospheric boundary layer, mainly because of its limited ability to account for the dynamics that are not explicitly resolved in the simulations. The goal of this research is to address those limitations in order to make LES a more reliable tool for the study of exchange processes.

These researchers focused on developing new subgrid-scale models to better represent the physics of the sub-grid scales and their effect on the LES results. This was done through the combination of field experiments and extensive numerical simulations. A critical factor in making fundamental progress in LES modeling was access to more powerful computers, which allow the researchers to increase the resolution and/or speed of the simulations. The resources at the Supercomputing Institute provided the computer power for high-resolution simulations needed to carry out cutting-edge research in the area of large-eddy simulation of turbulent flows.

The researchers also used the visualization software at the Supercomputing Institute to create movies of the three-dimensional transient temperature and water vapor fields in the boundary layer. These movies allowed them to gain insight into the dynamics of the simulated flow and its sensitivity to changes in the sub-grid-scale models and boundary conditions. ■

Research Group and Collaborator

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Industrial and Environmental Flows

This research group is studying the development of large-scale flow computation methods and computer codes for scientific and engineering applications. Their objectives are to advance the state of the art of computational fluid dynamics and to promote its applications to industrial and environmental problems through the development of:

- Improved governing equations and boundary conditions
- Improved modeling techniques and numerical schemes

In the first area, the group has 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 also accurately calculate highly time-dependent flows that cannot be computed with the incompressible flow approach. The research group also developed a virtual single phase flow model for the simulations of naturally-occurring cavitating flows.

In the second area, the researchers developed a general four-dimensional vector approach to simulate time-dependent three-dimensional flow. With this approach, it is possible to obtain a very accurate computation method for solving problems involving very rapid grid movement and deformation. The group is also developing a fully compressible two phase flow model for ventilated supercavitating flows. They have found that the treatment of the equation of continuity, which embodies the compressibility effect, is the key to simulating cavitating flows. ■

Research Group and Collaborator

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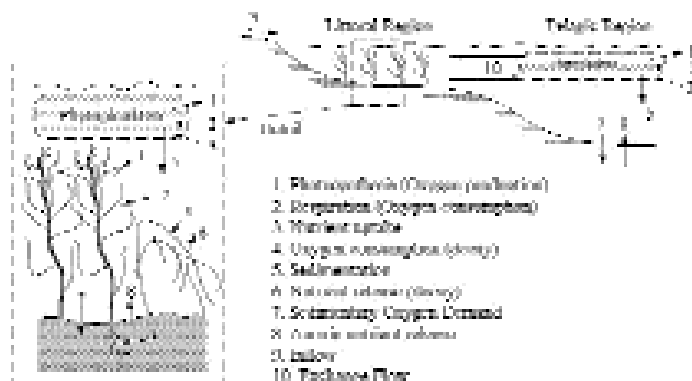
Quantifying the Uncertainties of Climate on Streams and Lakes

This research group's long-range goal is to estimate the potential effects of climate and climate warming on streams and lakes, specifically water quantity, water quality, and fish habitat. Specific aims of recent research have been:

- To establish potential upper bounds on stream temperatures based on physical principles and stochastic analysis
- To investigate the stochastic imprint of climate/weather in stratified lake temperatures
- To refine the relationship between fish habitat and climate in streams in the United States
- To develop a model for macrophyte (plant) growth in the littoral regions of lakes in response to climate/weather parameters, and to couple it to lake water quality

In the first area of research, the group used a statistical method to arrive at an upper bound on weekly stream temperatures. There are physical reasons for believing that stream temperatures will not rise indefinitely when the projected climate warming occurs. The group analyzed temperatures recorded at 993 United States Geological Survey (USGS) stream gauging stations throughout the United States, and computed a maximum series for each gauging station, plus an enveloping standard deviate, K . The K -values were analyzed to look for trends with respect to record length and geographic patterns. The group compared observed maximum stream temperatures with predictions using various K -values for all streams. K between 6 and 7 was found to give predictions that correlate well with the observed maxima.

In the second research area, this group analyzed water temperature time series data from two thermistor chains in a small Minnesota lake. Water motions in lakes are frequently energized by wind and heat exchange at a lake's surface. Heat exchange with the lake sediments and inflows/outflows can also be important, for



Biogeochemical and transport processes in the littoral and pelagic regions of a lake.

example if the lake is covered with ice. The energy input from these sources lead to currents, internal waves, convective circulation, and turbulence. The cumulative interactive effects can be seen in the temperature stratification dynamics of a lake with depth.

Individual effects of these processes appear as periodic or random components imprinted on the water temperature time series and can be extracted by stochastic analysis. The group used the analysis of their data to illustrate the stochastic characteristics of the water column response to external forcing.

A significant variability of the water temperature response with depth and season was determined from the thermistor chain records using autocorrelation and spectral density functions. The characteristics of the autocorrelation and spectral density functions clearly indicate a four-layer stratification structure that parallels the structure conventionally derived from spatial temperature gradients. Near the surface (surface mixed layer) diurnal periodicities, presumably due to daily heating and cooling, are dominant and mesoscale periodicities related to the passage of weather systems are evident. Near the thermocline, strong periodicities with high amplitudes due to natural internal waves are formed. In the deep parts of a lake

Heinz G. Stefan, Associate Fellow

(hypolimnion), sources of organized fluctuations are mostly absent. There is also evidence of a benthic layer in the bottom-most one to two meters of the lake that is distinguished by larger amplitudes and low frequencies. Overall, the water temperature spectrum is the result of the superposition of periodic phenomena with variable frequencies and phenomena with high intermittency. The results show that stochastic imprints/characteristics of water temperature change with time, and can be used to characterize the stratification structure in a lake based on temperature dynamics in addition to the conventional characterization (epilimnion, metalimnion, hypolimnion) based on mean spatial (vertical) temperature gradients.

This group also studied the suitable thermal habitats of 57 fish species to project potential habitat changes under global warming; to accomplish this, they analyzed data from 764 stream gauging stations in the contiguous United States. Global warming was specified by air temperature increases projected by the Canadian Centre of Climate Modelling General Circulation Model for a doubling of atmospheric CO₂. The aquatic thermal regime at each gauging station was related to air temperature using a nonlinear stream temperature/air temperature relationship.

Suitable fish thermal habitat was assumed to be constrained by both maximum temperature and minimum temperature tolerances. For cold-water fishes with a 0 °C lower temperature constraint, the number of stations with suitable thermal habitat under a 2xCO₂ climate scenario is projected to decrease by 36%, and for cool-water fishes by 15%. These changes are associated with a northward shift of the range. For warm-water fishes with a 2 °C lower temperature constraint, the potential number of stations with suitable thermal habitat is projected to increase by 31%, i.e. associated with a northward range extension.

A current emphasis of the water-quality modeling project considers the coupling of rooted aquatic plant (macrophyte) growth to biological, chemical, and physical processes in lakes. Mechanistic relationships are being developed for macrophyte production, respiration, senescence, and decay, and for the subsequent effect on dissolved oxygen, carbon, and nutrient balances in the littoral zone water column. The process formulations will be combined with laboratory and field data to produce a calibrated model that will be used to study the sensitivity of water quality variations to macrophyte parameters at daily to seasonal time scales.

A macrophyte growth model has been developed to calculate the rate of production of rooted aquatic macrophytes as a function of basic physiological parameters (growth and respiration rates) and controlling physical parameters (incident irradiance, water temperature, light attenuation). The model is developed to be general, rather than specific to a particular species, with the intention of broadly characterizing growth behavior as a function of a few key parameters. The growth equations are solved analytically using the assumption of uniform temperature and biomass over depth. The model includes expressions for instantaneous rate of growth and equilibrium biomass and set of dimensionless parameters are defined and used to characterize four growth regimes. Finally, transient growth behavior is being explored using both analytic and numerical integration.

Further research will include a process model to study the effects of macrophytes on water temperature, flow, turbulent transport, and sedimentation. Currently, this group is developing a model for turbulent transport processes within a macrophyte bed, a key component for modeling the coupling of macrophytes to the transport of dissolved oxygen, carbon, and other substances. The transport model includes the effect of macrophytes on turbulent diffu-

sion by estimating the drag forces on vegetation and the subsequent dampening of flow turbulence. ■

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Clustering Evaluation

This project includes three categories:

- Information retrieval
- Text document classification
- Optimal clustering

The group has developed a new weighting scheme for a vector space model to improve retrieval performance for an information-retrieval system. The main idea of this approach is to consider not only present terms but also absent terms in finding similarities among document vectors. Optimal clustering, in this research, will provide hierarchical clustering algorithms with a clustering criterion. This criterion is based on the centroid approach and the squared error method that have been the most widely-used evaluation measures for clustering techniques. The group's approach will be demonstrated and verified using the uncertainty of clustering optimality. By applying this feasible clustering criterion to document classification, the group will obtain multiple optimal centroids, which will reduce classification errors. ■

Research Group and Collaborators

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Data Mining: Discovery of Information in Large Datasets

The problem in mining hidden associations present in large amounts of data has seen widespread applications in many practical domains such as customer-oriented planning and marketing, telecommunication network monitoring, and analyzing data from scientific experiments. The combinatorial complexity of the problem and phenomenal growth in the sizes of available datasets motivate the need for efficient and scalable parallel algorithms. The design of such algorithms is challenging. This research group has presented an evolutionary and comparative take on many existing representative serial and parallel algorithms for discovering two kinds of associations. It was shown that many existing algorithms actually belong to a few categories that are decided by the broader design strategies. Overall, the aim of this research was to provide a comprehensive account of the challenges and issues involved in effective parallel formulations of algorithms for discovering associations, and how various existing algorithms try to handle them.

A new project by this group involves using data mining to predict the observed properties of chemical compounds. More specifically, the researchers' goal is to predict the impact sensitivity of energetic materials. The group used different types of chemical information for this project, including information from computational chemistry simulations and general chemical information—especially structural information—available in chemical databases such as the Cambridge Structural Database. ■

Research Group and Collaborators

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Optimal Clustering and Its Application; Data Space Dimensional Reduction for Support Vector Machines

This group's first project was divided into two categories: text document clustering and classification. The clustering technique provided hierarchical clustering algorithms with a stopping criterion. This criterion was based on the centroid approach and the squared error method, which have been the most widely used evaluation measures for clustering techniques. The approach was demonstrated and verified using the traditional concept of entropy. The researchers interpreted clustering as a seeking process that finds a data configuration containing the minimum clustering entropy. Since a hierarchical clustering algorithm tries to find a clustering configuration that approaches to the optimal, the number of clusters in the configuration was supported by the partitional clustering algorithms in order to perform the best clustering. The clustering performance was then evaluated by and compared to the optimal configuration found by combinatorial search. By applying this clustering criterion to classification, each class was segmented to have multiple centroids. As the centroids then provided more precise information for the internal configuration of the class, it was expected that this clustering approach would support classification to reduce the classification error. The researchers used supercomputing resources to perform their combinatorial searches and massive tests.

The researchers in this group have also begun a project to investigate sampling methods for data mining. Three methods were 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. ■

Research Group

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pARMS: 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 the 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 of the preconditioning techniques available in its predecessor (PSPARSLIB) as well a new class of methods that are based on recursive algebraic multilevel techniques.

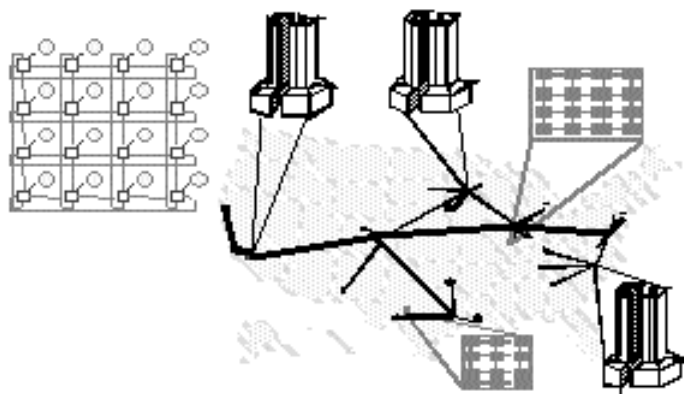
The group recently issued a technical report to illustrate the performance of the package. The package is also now available to the public. The researchers will now continue to develop other domain decomposition-type preconditioning techniques, and they will use pARMS to solve realistic scientific and engineering problems. ■

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The iScheduler: A Synergistic Approach to Scheduling Computational Science Applications



Integrated scheduling in a grid.

Efficiently executing resource-intensive parallel scientific applications in dynamic parallel and distributed production environments is a challenging problem. Applications can experience large slowdowns or high wait times due to contention for these limited valuable resources especially as the scale of the application grows to realistic sizes. While the performance problems are rooted in the oversubscription of system resources, they are further exacerbated by inefficient resource utilization both by the system and the application. The problem is that application schedulers typically select resources without regard for the negative impact this may have upon other applications and may even over-allocate resources with limited benefit. In contrast, most job schedulers in parallel systems are often designed to optimize metrics that may not deliver the best possible application performance, but offer good average performance or favor machine utilization.

These researchers are investigating a new paradigm that narrows the functional gap between job and application scheduling called integrated scheduling or iScheduling. The goal of iScheduling is to exploit the advantages of job scheduling (global view of competing appli-

cations) with application scheduling (specific knowledge of an application) to yield reduced time-to-solution for computational science applications and make more efficient use of available hardware for high performance systems. Within the iScheduler, resource allocation decisions are more fluid than in most static scheduling systems. To achieve this, the iScheduler and application interact using an interface that provides dynamic application performance information to the iScheduler (sensing) and an interface that is used to control the application's behavior and resource usage in response to information gathered by sensing (actuating). The researchers are establishing the efficacy of iSchedulers by building several instances and evaluating their performance on computer clusters. ■

Research Group

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Modeling of Vertical Lasers; Integrated Optical Circuits; Linearized Optical Modulators

This research group developed a self-consistent model of the Vertical Cavity Surface Emitting Laser. They 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. They are modifying this code to do the vector solutions.

The group continued their work on integrated optics, integrated switch structures using semiconductor laser amplifiers as the switch elements, integrated semiconductor laser amplifiers with Faraday rotation isolation, dielectric waveguide amplifiers, and dielectric waveguide amplified spontaneous emission sources. All these devices require waveguide mode solvers, with and without gain/loss, and in the case of the Faraday rotation isolator, anisotropic media.

A new, related area of research begun this year involved linearized optical modulators. These modulators provide high optical index of modulation for optical communication systems. The researchers designed the modulators by using the directional coupler with variable coupling. The spatially varying coupling function can be obtained by the Fourier transform technique. However, a more accurate coupling function can be obtained by the iterative Gelfand-Levitan-Marchenko method, which requires an efficient calculation tool. The researchers are using Supercomputing Institute resources to run the MATLAB and MATHEMATICA programs needed for these calculations. ■

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Calculation and Analysis of EM Field in MRI

Magnetic resonance imaging (MRI) causes electromagnetic fields that run through patients. This research group's specific area of interest is MRI used on patients with a deep brain stimulation (DBS) system implanted. There is some fear that a radio frequency (RF) field pulsed sequence used in conjunction with MRI for imaging DBS could cause sufficient current flow in the DBS microelectrode lead to cause tissue damage.

This project formed a preliminary step to determine the current flow in this lead. Sample data was taken for the electromagnetic (EM) field distribution in patients without DBS in the MRI. The EM field distribution was then calculated using the Maxwell Software Package from Ansoft. This calculation will be compared to theory and experimental data, which in turn will be used as a building block to determine current flow induced from pulsed sequences in DBS leads from MRI. ■

Research Group

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Electrical-Magnetic Field Simulation for Micro-Optical Elements

This research group investigated 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. This group applied the rigorous-coupled-wave (RCW) method to simulate three-dimensional periodic micro-optical elements (i.e., micro-lens arrays, gratings, and so on) and achieved good results. With mass transport technology, the group was able to fabricate various micro-optical elements so that they could compare a computer model with experimental results. Given sufficient computational resources, the current model handled many realistic structures. However, to simulate more complex structures, a three-dimensional non-periodic model proved necessary. These researchers continued to improve their current model and develop a three-dimensional model to simulate some interesting micro-optical structures. Computational results were compared with experimental measurements. Finally, the group simulated elements, such as optical read-out head, near field microscopy, and micro-ellipsometry. ■

Research Group

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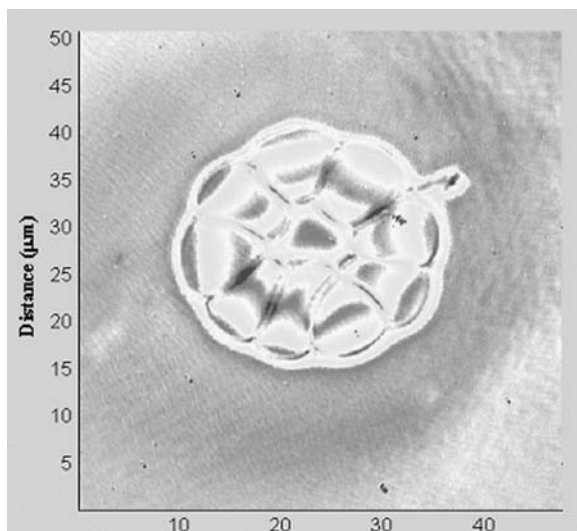
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Polarization ratio image of human red blood cell cluster formed by nine red blood cells. This image is taken by an imaging ellipsometer. The contrast comes from the variations of thickness and refractive index of the sample.

David J. Lilja, Fellow

Simulating New Types of Computer Architectures

These researchers investigated architectural tradeoffs for future processor designs. For this work, the group used a detailed execution-driven simulator with the SPEC CPU 2000 benchmark programs (see www.spec.org). Due to the computationally intensive nature of the simulator and the large input sizes of the current SPEC benchmark programs, this research used the computing and memory resources of the Supercomputing Institute Origin and SP supercomputers.

In building new generations of microprocessors with ever-higher performance, CPU designers always face two major challenges. The first is to tackle the scalability issue when increasing the number of instructions issued per machine cycle while simultaneously shortening the clock cycle time. The second challenge is to bridge the worsening “speed gap” between the processor and its memory. Previously, the group proposed the “superthreaded” processor architecture in order to address these challenges by exploiting more sources of parallelism in application programs through both instruction-level and thread-level speculation with compiler-assisted cross-thread runtime data dependence checking.

One of the main goals of this project was to develop new compiler technology needed to support the superthreaded architecture. Preliminary results showed excellent potential for reducing application execution time with this architecture, but they also highlighted the need to deal more aggressively with the memory latency problem. In this group’s more recent work, the researchers developed a processor simulator to help validate the superthreaded architecture.

To address one aspect of this goal, the researchers focused on the use of high-performance computing in speculative multithreading. Very large-scale integration (VLSI) transistor densities now allow entire systems to be built on a single chip. However, smaller

improvements in processor clock speeds force processor designers to exploit exotic techniques to improve performance. The superthreaded processor architecture was developed with the expectation that this would improve the performance of application programs that are difficult to parallelize using traditional approaches. This new architecture is a hybrid of a high-performance microprocessor, such as the Intel Pentium, and a multiprocessor, such as the SGI Origin. Unlike these traditional systems, however, this approach relies heavily on speculation in which the processor “guesses” which instructions the program will execute next. Run-time verification ensures that the compiler’s speculation was correct. A special operation was executed to fix the processor’s state if the speculated outcome was wrong. The researchers developed a detailed, cycle-accurate simulator of the superthreaded processor to evaluate its performance potential. This simulator actually executes any application program that has been compiled using an integrated parallelizing compiler. While executing the application program, the simulator estimates the number of cycles that an actual superthreaded processor would require to execute the program. The simulator allows the designer to vary the number of thread processing units, the capabilities of each unit, and other important parameters.

Another area of interest included compiler-assisted sub-block reuse. The fact that instructions in programs often produce repetitive results has motivated researchers to explore various alternatives to exploit this value locality, such as value prediction and value reuse. Value prediction improves the available Instruction-Level Parallelism by allowing dependent instructions to be executed speculatively after predicting the values of their operands. Value reuse, on the other hand, attempts to remove redundant computations by buffering the previously produced results of instructions and skipping the execution of instructions with

repeating inputs. Previous value reuse mechanisms used a single instruction or a naturally formed instruction group, such as a basic block, a trace, or a function, as the reuse unit. These naturally formed instruction groups are readily identifiable by the hardware at run-time without compiler assistance. However, the performance potential of a value reuse mechanism depends on its reuse detection time, the number of reuse opportunities, and the amount of work saved by skipping each reuse unit. Since larger instruction groups typically have fewer reuse opportunities than smaller groups, but also provide greater benefit for each reuse-detection process, it was found to be very important to find the balance point that provides the largest overall performance gain. To this end, these researchers proposed a new mechanism called sub-block reuse to intelligently group instructions into reuse units using compiler-assistance. The goal was to balance the reuse granularity and the number of reuse opportunities. The sub-blocks were produced by slicing the basic blocks at compile-time using appropriate dataflow considerations. The simulations with the SPECint95 benchmarks showed that sub-block reuse with compiler assistance has a substantial and consistent potential to improve the performance of super-scalar processors with speedups ranging from 10–22%.

The researchers also developed a complexity-effective verification technique utilizing the Cray SV2 Cache Coherence Protocol. In this instance, modern large-scale multiprocessors, capable of scaling to hundreds or thousands of processors, have proven to be very difficult to design and verify in a timely manner. In particular, the verification process (i.e., proving that the design is functionally correct), is often the most time-consuming aspect of developing the system. The group also proposed a method of dealing with the verification complexity of a directory-based coherence protocol, providing

the framework for a methodology that is built on a formal model of the coherence protocol, a language, and the register transfer language (RTL) implementation. This approach was used to verify the SV2 directory-based coherence protocol. ■

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P. Paul Ruden, Associate Fellow

Properties of Semiconductor Devices and Materials

These researchers calculated the electronic structure and related properties of semiconductor materials and novel devices. Under previous Supercomputing Institute grants, this group's work focused on calculations of the electronic structures of quantum wires, on transport simulations for large band-gap III-nitride materials using Monte Carlo techniques, and on the modeling of strain effects in III-V heterostructure devices in the framework of the finite element method.

Having recently developed iterative, two-dimensional and three-dimensional finite element codes for thermal modeling of III-nitride device heterostructures, the research group sought to avoid the crude simplifications usually adopted for this problem. In particular, their method can handle the different temperature dependencies of thermal conductivities of the substrate, the active material, and the metal contacts in a hybrid device structure. Because of the large computer time and memory requirements of the three-dimensional finite element code, access to the multiprocessor machines with large memory capacity was critical for these studies.

Additional work focused on further Monte Carlo transport simulations for large-band-gap materials and on the creation of device models for large gap semiconductor devices. This last topic required significantly higher levels of precision than conventional semiconductor device modeling, primarily due to the much wider range of values assumed by variables such as the electron and hole concentrations.

The group is also considering the use of altogether new materials, based on organic compounds. ■

Research Group and Collaborators

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Tri- and Multi-Linear Methods for Signal Processing in Communication Engineering

This group is conducting research on tri- and multi-linear 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, chromatographic, 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 principle 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 also developing efficiently-fitting algorithms for the PARAFAC model and derivatives/generalizations. ■

Research Group

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Micromagnetic Simulations Including Thermal Fluctuations

Current magnetic recording technology has approached several new technical barriers that may limit the further increase of hard disk recording density. Examples of these barriers include fundamental limitations in the thermal stability and switching speed of the magnetic domains. Instead of the current longitudinal recording method, one of the alternatives has been to record the media perpendicularly, which, however, may require significant technological changes.

These researchers have developed a micromagnetic model that simulates the characteristics of perpendicular recording media and recording heads, and have already demonstrated the accuracy of the media simulation. They are now using the model to solve two important problems. The first is the prediction of hysteresis loops for materials exhibiting defects and strongly exchange-coupled grains. The second problem is the design of a recording head that can develop adequate field, gradient and switching speed to be useful at densities of a terrabit/inch². Both of these problems require large computational resources either because the sample region must be finely divided (the media problem) or because the sample region must be relatively large (the head problem).

Another, related topic of research for this group is micromagnetic predictions of bit decay caused by thermal fluctuations over long time scales. Thermal decay in magnetic recording media increases with time, consequently decreasing the signal-to-noise ratio. The new scaling technique was used to predict bit decay over long time scales. An ideal square-wave field was used to record bits in thin film magnetic recording media. Comparison of bit thermal stability for longitudinal and perpendicular thin film media with similar K_uV/kT was carried out at recording densities from 50 to 400 Gbit/in². Bit decay in a Co/Pd superlattice film at ~80 Gbit/in² was studied as well. ■

Research Group

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William Seyfried, Jr., 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 were required. Moreover, to better understand the conceptual framework for experimental data, molecular dynamic calculations were needed. The combination of experimental and theoretical constraints go a long way toward understanding phase relations involving quartz in sub-seafloor hydro-thermal systems. ■

Research Group

Dionysios I. Foustoukos, Graduate Student Researcher

David A. Yuen, Fellow

Numerical Simulations of Geophysical Phenomena

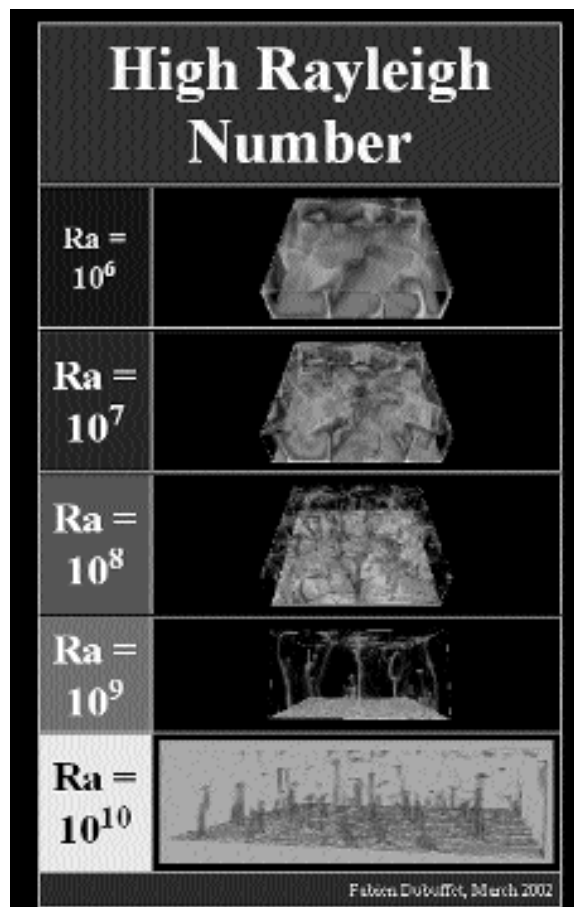
These researchers worked on several large-scale computational problems that required both the speed and memory resources of vector and massively parallel computers. Some of the most significant problems addressed by this group were the following:

- Three-dimensional mantle convection with variable thermal conductivity and viscosity
- Mixing dynamics in convection
- Molecular dynamics and dissipative particle dynamics as applied to multiphase flow with 10^7 particles
- Visualization of large data sets
- Numerical modeling of the Earth's lithosphere-mantle system with complicated physics and rheology
- Three-dimensional convection in a spherical shell

The following provides an overview of some of the work performed by this group.

One area of interest for this group is secondary upwelling instabilities developed in high Rayleigh number convection. In this area, possible applications to hot spots were observed through conducted numerical experiments for mantle convection in an axisymmetrical spherical-shell geometry from Rayleigh numbers ranging from three million to ten billion for a purely basal heating configuration. For Rayleigh numbers between around 30 million and one billion, a string of these secondary instabilities can develop from a single plume. Analysis of the spectrum of wavelength associated with the fold instabilities showed that there is a window in the Rayleigh number between around ten million and one billion where these secondary folding instabilities would develop. These results, when applied to the upper mantle, may explain the formation of hotspots in a turbulently convecting upper-mantle with a Rayleigh number greater than ten million.

This group also studied dissipative particle



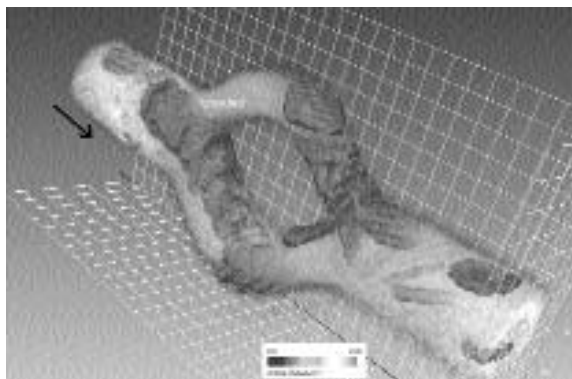
High Rayleigh number three-dimensional convection for the Earth's mantle from Rayleigh number 10^6 through 10^{10} with the highest resolution of $601 \times 601 \times 601$ grid points.

dynamics (DPD). DPD and its generalization—fluid particle model (FPM)—represent the “fluid particle” approach for simulating fluid-like behavior in the mesoscale. Unlike particles in the molecular dynamics method, the fluid particle can be viewed as a “droplet” consisting of liquid molecules. In FPM, fluid particles interact by both central and non-central, short-range forces with conservative, dissipative, and Brownian character. This group discovered that the efficiency of the FPM code depends strongly on the number of particles simulated, geometry of the box, and the computer architecture. This FPM code can be

applied for simulating mesoscopic flow dynamics in capillary pipes or critical flow phenomena in narrow blood vessels.

Another project for this group involved developing a method for data mining. Current advances in computer hardware, information technology, and data collection techniques have produced very large data sets in a wide variety of scientific and engineering disciplines. The group implemented a map-like approach to retrieve useful information from geophysical and geological data: spatial data is mapped onto a two-dimensional grid from which the user can quiz the data with the map interface as a user extension. The data is stored on the server, while the computational gateway separating the user and the server can be the front end of an electronic publication, an electronic classroom, a survey, or an e-business. The group used a combination of JAVA, JAVA3D, and PERL for processing the data and communicating between the user and server. The user can interrogate the geospatial data over any particular region with arbitrary dimensions and then receive back relevant statistical analysis, such as histogram plots and local statistics. The group has used this method for distribution of prime numbers, two-dimensional mantle convection, three-dimensional mantle convection, high-resolution satellite reflectance data over multiple wavelengths, and molecular dynamics describing the flow of blood in narrow vessels.

Other topics of study for this period included: the problem of viscoelastic relaxation of the earth solved by a matrix eigenvalue approach based on discretization in grid space; rheological structure and deformation of subducted slabs in the mantle transition zone with implications for mantle circulation and deep earthquakes; and modeling of viscoelastic plume-lithosphere interaction using adaptive multi-level wavelet collocation method. ■



Blood cells clotting in bifurcating capillary vessel simulated by using discrete particles. The blood cells are modeled by particles on strings. The plasma fluid is represented by a fluid particle model. Plasma velocity is the lowest at the choking point. The vessel diameter is 15–20 micrometers and the hematocrit is 10%. The Reynolds number, Re , is approximately 0.01. This simulation used two million particles, and was created using the AMIRA package.

Research Group and Collaborators

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Mathematical Model of Human Atrial Fibrillation; Two-Dimensional Guillotine and Non-Guillotine Cutting Stock Problems

This research involved the study of electrophysiology in the heart. Specifically, it centered in the spatial propagation of waves of electrical activity occurring in normal and diseased hearts with a view toward exploring various therapeutic strategies such as tissue ablation, electrical defibrillation, and pharmacological treatments.

An object-oriented approach was adopted in order to attempt simulation of electrical activity in the entire human atria using detailed biophysical models of atrial cell electrophysiology. A sound numerical time-integration scheme with backward-differentiation time-stepping, a modified Newton nonlinear solver, and an iterative linear solver were all used along with an explicit integrator. Parallel versions of these codes were implemented on the Origin 2000. A parallel version was tested on the IBM SP using a beta-version c++ compiler.

These models were supplemented by finite element models of radio-frequency ablation of atrial tissue as well as boundary element models of sensing of electrical activation using leads currently under research at Medtronic.

The use of mathematical models in the design of therapies holds considerable promise. With detailed information on the effects of genetic mutations on protein function, the ability to incorporate such data into cellular models, and better models of the action of drugs on cellular processes, the researchers found themselves in a position to reconstruct the function and disease of human organs and to explore therapeutic strategies.

This research group continued to investigate ways to find stock-cutting patterns so that order demands are not exceeded and waste is minimized. The group developed and coded several algorithms for solving various two-dimensional cutting stock problems. The methods include simulated annealing technique

and an integer programming approach. The large size of realistic problems required the use of the Supercomputing Institute's resources. ■

Research Group

Anton Leykin, Graduate Student Researcher

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Computational Aspects of Analytic Number Theory

This research group continued its computational analyses of high frequency eigenfunctions of the Laplacian (for fuchsian groups). These jobs were run in Sweden on a Cray-T3E and Cray YMP-EL. Files held and codes derived from work performed at the University of Minnesota play a vital role in the analysis. The group has calculated the value distribution properties as well as local moments of “CM-forms,” a special kind of eigenfunction of the Laplacian. They are determining if there will be statistical anomalies visible when passing from a generic to “almost deterministic” setting. The group also considered the statistical properties of Fourier coefficients of automorphic forms on non-arithmetic Hecke groups and related groups of congruence type.

Most recently, the group has been exploring Maass waveforms of CM-type on subgroups of the modular group $SL(2, \mathbb{Z})$. They have computed correlation coefficients for a multitude of 1-dimensional “cross-sections” and have found a very interesting oscillatory pattern in this, which seemingly ties in with work of M. V. Berry (in the Euclidean case). The group will be exploring this further, including for fully random (pseudo) Maass waveforms. ■

Research Group and Collaborator

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John S. Lowengrub, Fellow

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

This research group is studying topological transitions and singularities of interfaces in fluid flows and biological systems. They use a dual approach of sharp and diffuse interface methods and are developing accurate and efficient algorithms. In fluid systems, they are investigating ternary fluid flows in which two of the components are immiscible but the third component is miscible with at least one of the other components. They are also continuing to perform high resolution simulations of droplet coalescence and break-up. In crystals, the group is studying the evolution of three-dimensional crystals with isotropic and anisotropic surface tension. In biological systems, the group is studying the morphology of non-necrotic vascular tumors.

In their fluid flow work, the researchers developed modelling pinchoff and reconnection methods for use in a Hele-Shaw cell. The group analyzed two diffuse interface models, called the HSCH model and BHSCH model, to study pinchoff and reconnection in binary fluid flow in a Hele-Shaw cell. In the HSCH model, the binary fluid may be compressible due to diffusion. The BHSCH model uses a Boussinesq approximation and the fluid is incompressible. Having found that the break-up of an unstably stratified fluid layer is smoothly captured by both models, the researchers concluded further that the HSCH model seems to be more diffusive than the BHSCH model and predicts an earlier pinchoff time, which causes subtle differences between the two in the pinchoff region. Away from the pinchoff region, both models yield nearly identical results and were demonstrated in convergence with the classical sharp interface model as the interface thickness vanishes.

These researchers also focused on producing boundary integral methods for multicomponent fluids and multiphase materials. As part of this research, the group participated in the

development of methods that accurately and efficiently include surface tension on the Kelvin-Helmholtz and Rayleigh-Taylor instabilities in inviscid fluids; the generation of capillary waves on the free surface; and problems in Hele-Shaw flows involving pattern formation through the Saffman-Taylor instability, pattern selection, and singularity formation.

In crystals, the group is studying the important question of 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. Linear analysis suggests that under certain conditions, the morphology of growing crystals may be controlled. The researchers confirmed this with their numerical experiments. They have developed a fully developed, three-dimensional boundary integral method to solve the diffusional evolution of interfaces. They began with isotropic surface tension, and have begun to extend their results to anisotropic interface kinetics.

In their research on tumor growth, the group is working to determine the conditions under which tumors become spherical or tend to break up, increasing the danger of spreading their cells throughout the body. They are using a model that couples a reaction-diffusion equation for nutrient with a Darcy's law for tumor motion. The model contains a surface-tension-like term that mimics the cell-to-cell adhesiveness. The resulting system is very similar to that describing motion of fluid in a Hele-Shaw cell. In the evolution process, competition arises between the growth/shrinkage of the tumor due to food supply and the stabilizing effect of the cell-to-cell adhesive forces. The group has performed linear analysis and developed boundary integral methods to solve the problem in two dimensions. ■

John S. Lowengrub, Fellow

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Nicolas Versluis, Research Associate

Xiaoming Zheng, Research Associate

Hua Zhou, Research Associate

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Computation of Active Martensitic Thin Films

This research group used supercomputing resources to numerically simulate temperature and stress-induced austenitic-martensitic phase transitions, as well as to investigate their use in active thin films and micromachines. Nonlinear, time-dependent partial differential equations that are numerically integrated present a novel challenge to computational science since the linearization of the model is not well posed. This ill-posedness manifests itself in the nonlinear computational model by the development of microstructure.

The researchers continued to investigate the influence of surface energy on the numerical solutions. The future goal of these computations will be to contribute to the understanding of the shape-memory effect and to make possible new applications of these materials in technology.

Another area of interest for these researchers was the stability of microstructure for general martensitic transformations. A general theory was developed for the stability of the laminated microstructure for martensitic crystals. The underlying theory was applied to the orthorhombic to monoclinic transformation, the cubic to tetragonal transformation, the tetragonal to monoclinic transformation, and the cubic to orthorhombic transformation. ■

Research Group and Collaborators

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Mathematical Modeling of Vertebrate Limb Development

A new model for limb development that incorporates both 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, has been previously developed. 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 and, because growth is explicitly incorporated, it was found that 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.

Recent research revealed details of the biochemical mechanism of differentiation at the molecular level. The team's future work intends to:

- Modify the existing model to incorporate new molecular information about the mechanism of limb development
- Extend the solution domain to four dimensions (3 spatial + time) to enable a realistic simulation of the limb development process

The aim of this project is to provide 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. ■

Research Group and Collaborators

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Steve Webb, Research Associate

Avram Bar-Cohen, Principal Investigator

Thermal Management of Micro/Nano Systems

This research focused on the next generation packaging, Single Level Integrated Module (SLIM). Previous studies were performed in two-dimensional and three-dimensional modeling of SLIM. The fine features of SLIM were modeled utilizing the extensive computing resources provided by the Supercomputing Institute. The features were expected to get finer and the enhanced computing power of the supercomputer is expected to solve this problem.

This group also used supercomputing resources to create a compact model of heat sinks. Inspiration for the current research derives from a possibility for modeling a detailed heat sink when treated as a porous block. The huge decrease in computational time in the compact model was the inspiration for this project. ICEPAK is the computational fluid dynamics tool used for modeling the compact heat sink model.

Another area of research concerned analysis of deoxyribonucleic acid (DNA) substrate's thermal behavior by using numerical approach. The numerical result was compared to experimental results, and the substrate's thermal profile was analyzed by ANSYS.

Further research is underway reviewing analytic expressions for heat transfer in natural convection from isothermal rectangular plates at various angles of inclination. Correlations are available which deal with both horizontal and vertical configurations, as well as recommended approaches for modifying the correlations to deal with inclined plates. The research group used Supercomputing Institute resources to conduct a numeric study of inclined plates in natural convection to examine the range of angles where the modified vertical and horizontal correlations are applicable. ■

Research Group

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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 widely used in recent years.

This research group is using the commercial software product ANSYS to develop a three-dimensional finite element model mimicking the clinical situation of prostate cryosurgery. The input for the model is patient-specific data. The model will also include an injury model to predict the tissue damage with known thermal history. This numerical model can be used to optimize the probe positions and the treatment time to ensure complete killing of the disease tissue while saving as much of the healthy surrounding tissue as possible. This model will be a very useful tool for pre-treatment planning of cryosurgery of the prostate, and will also be very useful for understanding the injury mechanism of cryosurgery. ■

Research Group

Xiaoming He, Graduate Student Researcher

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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 temperature. Some of these reactions are desirable; others are unwanted. For example, corona-enhanced chemical vapor deposition 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 study was to model the corona plasma and the global gas phase reaction that is the rate-limiting step in the deposition process. The first step was to obtain the electron density and energy distributions in the plasma. Electron density was obtained from a simplified set of Maxwell’s equations and Ohm’s law. The electron energy distribution function was obtained from the Boltzmann equation. These values were used to determine the rate of production of precursors. The concentration distribution and flux of the precursor to the discharge electrode surface were then determined from solutions of the governing fluid dynamic and mass transfer equations. Lastly, this model was used to determine the impact of various operating and geometric parameters of deposition rate. ■

Research Group

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Large-Scale Simulations of Turbulent Reacting Flows

The objective of this research is to perform numerical simulations of turbulent reacting flows via the combination of large eddy simulation (LES) and reduced chemical kinetics. There are two major issues that must be resolved to facilitate LES of turbulent reacting flows:

- Construction of an efficient numerical scheme for solving the governing transport equations
- Implementation of a chemical kinetic mechanism that can accurately capture the chemistry of complex hydrocarbon flames

In this work, both direct numerical simulation and LES were performed. With this approach, the researchers assessed the performance of the reduced mechanisms and the numerical solution procedures. LES is facilitated by introducing the “filtered density function” (FDF), and by providing an effective numerical means to simulate this FDF. Because of the added dimensionality of the compositional variables, solution of the FDF transport equation by conventional numerical methods is possible in only the simplest of cases. However, a Monte Carlo method may be used for this purpose. The use of these schemes has proven very effective in Reynolds averaged Navier-Stokes simulations. Considering the capabilities of the scheme—and encouraging results in preliminary usage of this scheme—an element of the research requires full utilization of this methodology for LES of turbulent reactive flows.

This project also involved plasma processing and plasma chemistry in three contexts of practical importance:

- Particle formation and transport in semiconductor processing systems
- Synthesis of nanostructured materials in a thermal plasma expansion process
- Fundamental studies of thermal plasma chemical vapor deposition

All of these projects involved the development of computer models in concert with ongoing experiments in the laboratory. Key issues included the detailed chemistry that governs film growth, and the nucleation, growth, and transport of particles in plasmas. ■

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Modeling Plasma Synthesis of Materials

This project involved plasma processing and plasma chemistry in three contexts of practical importance:

- Particle formation and transport in semiconductor processing systems
- Synthesis of nanostructured materials in a thermal plasma expansion process
- Fundamental studies of thermal plasma chemical vapor deposition

In the first area, the research group is developing approaches for modeling particle formation, growth, charging, coagulation, and transport for plasma processes used in the microelectronics industry to deposit and etch thin films. Particle contaminants in such systems lead to defects and poor product yield. The group has 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.

In the second area, the research group is studying nanophase materials, which show reduced sintering temperature, increased hardness, and interesting electronic and optical properties. The group has developed a process called hypersonic plasma particle deposition, in which reactants introduced into a high-temperature plasma are supersonically expanded through a nozzle. They have also developed a model for flow through the aerodynamic lens assembly that solves aerosol general dynamic equation and couples it to the fluid flow model. The developed model accounts for the effect of Brownian diffusion of particles. The next step is integrating the effect of particle diffusion into the model.

In the last research area, the group has begun investigating thermal plasma chemical vapor deposition of hard ceramic materials, particularly silicon carbide and boron carbide. The group has designed a completely new experi-

mental reactor and has developed models to predict the flow and temperature distributions in this reactor. ■

Research Group

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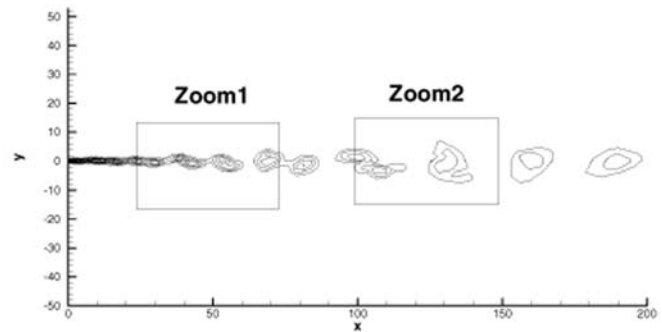
Computational Study on Heat Transfer in Nanofluids; Numerical Simulation of Instantaneous Energy Separation; Heat Transfer at High Rayleigh Number

The researchers considered the numerical simulation of instantaneous energy separation.

Instantaneous flow and total temperature field were numerically simulated to investigate the mechanisms of energy separation in shear and jet flows. The instantaneous pressure and temperature fluctuation within the flows provide information for understanding of the mechanisms of energy separation.

Another area of research involves heat transfer in gas turbines, which are widely used for power generation in industries. Since complicated geometries in gas turbines induce three-dimensional flow structure, heat transfer and fluid flow characteristics are not yet fully understood. In addition, computational fluid dynamics does not predict heat transfer and fluid flow correctly because of this complicated flow structure. Using the results of experimental and computational analysis, this group is constructing a numerical prediction model of heat transfer and realizing the limitation of heat transfer models in three-dimensional flow.

Further research involved the analysis of natural convection and heat transfer, which requires a high Rayleigh number. Flow and heat transfer systems at high Rayleigh number ($\sim O(10^{15})$) in a Benard convection cell were numerically simulated using a spectral/Chebyshev collocation method. The researchers identified Rayleigh numbers at which transitions in the behavior of Nusselt number occur, and then studied the mechanisms responsible for such transitions. ■



Vortex generation plot from shear jet.

Research Group and Collaborators

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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 better 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 was developed and modified during this group's study. These transport properties were then used to simulate the various processes mentioned above.

As a whole, the projects undertaken by this research group involved the iterative or transient solution of a large set of coupled non-linear equations, often with a very fine grid resolution in a two- or three-dimensional geometry, and therefore, required Supercomputing Institute resources. ■

Research Group

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Highly Realistic Modeling of Low-Pressure Processing Plasmas

These researchers studied new approaches for fast and realistic modeling of low-pressure processing plasmas. One focus was the accurate prediction of the electron 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 must use a number of approximations and are limited in their range of validity. The researchers used a highly realistic Monte Carlo approach based on first principles to accurately determine the electron energy distribution function in a low-pressure plasma. The results determined by the researchers provided new insight into the physics of electron transport processes, both in configuration and in energy space. The benchmark calculations performed also served as reference for comparisons with less general methods based on the approximate numerical solution of the Boltzmann equation.

A second focus of this research was the study of the chemical nucleation of nanometer-sized particles in plasmas. Here the researchers focused on the chemical nucleation of clusters in low-pressure silane plasmas. The formation of particles in low pressure plasmas was of high interest, both from the viewpoint of synthesis of new nanostructured materials and as it related to particle contamination in low pressure plasma processing of microelectronic devices. The formation of initial clusters should be understood as a sequence of reversible chemical reactions. This project continued to consider the development of a chemical reaction mechanism describing chemical clustering in low-pressure silane plasmas. The mechanism included neutral and ionic chemistries, particle coagulation, and transport modeling using aerosol dynamic methods. ■

Research Group and Collaborator

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Peng Zhang, Graduate Student Researcher

Thomas H. Kuehn, Fellow David B. Kittelson, Co-Principal Investigator

Modeling and Numerical Simulation of Megasonic Cleaning

The objective of this research team was to develop a model based on first principles to predict contaminant particle removal from silicon wafers in megasonic tank cleaning systems. Such a model could be used to design new generation cleaning equipment by varying parameters such as:

- Transducer shape, frequency, and power input
- Tank geometry, transducer location, and pumped flow conditions
- Wafer spacing, carrier design, and location
- Liquid temperature and dissolved gas concentration

The project included two parts. The first was to improve the model for the three-dimensional megasonic energy field in a specially-designed, well-instrumented megasonic cleaning tank. This type of tank is used to remove submicron particles from the surfaces of silicon wafers and electronic parts or to chemically process silicon wafers in a semiconductor manufacturing process.

The second part of the project was to correlate cleaning efficiency (particle contaminant removal) with the local sound density distribution, the microstreaming field, and cavitation intensity distribution. The modeling method, calculated results, and final report provided industrial users information for evaluating and improving megasonic cleaning systems. ■

Research Group and Collaborator

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Humberto Ortiz, Graduate Student Researcher

Yi Wu, Graduate Student Researcher

Ching-Hsu Yang, Graduate Student Researcher

Perry Y. Li, Principal Investigator

Optimization of Flow Forces in Hydraulic Valves; Numerical Experimental Platform for an Aquatic Vehicle Propelled by an Oscillating Foil

This research group was involved in two major areas of interest:

- A project to exploit fluid flow induced instability to enhance the dynamic response of electrohydraulic valves with limited solenoid actuation capability
- The investigation of the motion planning and control issues involved when an aquatic vehicle is propelled by an oscillating foil

In the first project, the researchers know that the geometric design of a valve affects both the unstable transient flow forces and the stable steady flow force. For their purpose, it is desirable to maximize the former and minimize the latter. The group is using the 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.

The second project involves the study of how vortex generation, propagation, and roll-up affect the dynamics of the aquatic vehicle. The facilities of the Supercomputing Institute are being used to run a numerical simulation platform that simulates the fluid flow, vortex interactions, and the dynamics of the aquatic vehicle. “Blob” (Rossi) codes in which vortex combinations are performed for efficient time stepping have been extended for this project. ■

Research Group

Brad Augustine, Graduate Student Researcher
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Benjamin Y. H. Liu, Principal Investigator

Monte Carlo Simulation of Particle Loading on Fibrous Filters

Air filters are used in a variety of industrial and commercial applications for removing aerosol particles from the air. In a typical filter, the dust particles are initially collected on the filter fibers both deep within the filter mat and also on the surface of the filter. As the dust loading progresses, the filter enters a loading regime where most of the particles are collected in the filter surface in the form of a dust cake. This condition is known as the “surface loading” or “cake filtration” regime. When the filter enters this surface loading regime, the resistance to flow increases rapidly, making it difficult for the fan or pump to maintain the required air flow rate through the system. In practice, when the flow resistance becomes high enough, the filter is either replaced or cleaned. It is in the interests of optimizing filter design to know when this transition to “surface” filtration occurs.

This research group is simulating the progressive loading of spherical particles onto fiber-like cylinders that constitute a simple model of a real fibrous filter. Particles are loaded onto the filter using a random Monte Carlo technique and the progressive growth of the particle layers is monitored to obtain an idea of the particle mass required for the filter as a whole to reach the transition condition. Filter fiber diameters, filter pore diameters, particle size distribution, and particle shape are varied to observe the influence of these parameters on the loading rate. Using this information, filter manufacturers can vary the parameters to optimally design their filters.

The group is using Supercomputing Institute resources to visualize the particle-loading process and to produce Web-based animations for subsequent analysis and presentation. ■

Research Group

Sho Takagaki, Graduate Student Researcher

Susan C. Mantell, Principal Investigator

Numerical Modeling of Thermoset Resin Composite Curing

An existing filament winding process model—using finite element software to predict fiber volume fractions, cure characteristics, temperatures, and pre-stresses induced during the filament winding process—was enhanced in this research in order to allow inclusion of autoclave curing of the composite and provide greater ease of use and versatility. The finite element analysis program ABAQUS, coupled with user-defined subroutines based on process sub-models, was used to perform this analysis. The model provided a useful analytical tool for the designer. The model could be used to optimize the fabrication of composite structures. ■

Research Group

Henry Jerome, Graduate Student Researcher

Peter H. McMurry, Associate Fellow

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

This research group created 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 $0.050\text{ }\mu\text{m}$, and perhaps as small as $0.015\text{ }\mu\text{m}$, will be critical to the yield of 1Gbit Dynamic Random Access Memory computer chips. Such ultrafine particles are typically produced by nucleation in the gas phase. The research group's main objective was to develop computational models to predict particle transport generated by nucleation in high-density plasma chemical vapor desposition tools.

During plasma processes, particles are charged negatively due to higher electron flux and trapped inside the plasma electrostatically. The purpose of this work was 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. ■

Research Group

Hiromu Sakurai, Research Associate

Suhas V. Patankar, Fellow

Computational Fluid Dynamics and Heat Transfer in Engineering Systems

The objective of this work is the simulation of fluid flow in domains with distributed resistances. These domains are characterized by having a large number of solid obstacles interspersed throughout the domain. These domains are found in many engineering devices such as heat exchangers, condensers, cooling towers, regenerators, and packed beds.

The numerical simulation is being conducted at large and small scale. The large-scale analysis is based on the distributed resistance method. Hence, the macro model is the entire device. The small-scale analysis is conducted on the micro model using a spatially periodic unit cell containing one or more solid obstructions.

The intent of the micro model analysis is to create a database of flow resistances for the macro model. Computations are made for a wide range flow angle and Reynolds number. The velocity distributions, obtained by solving the Navier-Stokes equations, are utilized to determine the local flow resistances.

In the macro model analysis, the continuum governing equations are solved to give the distributions of the velocity throughout the domain of interest. The field distributions are utilized in determining parameters of engineering interest such as pressure drop. ■

Research Group

Aiman Alshare, Graduate Student Researcher

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Nanoparticle Collision With a Surface

Filters are routinely used to remove toxic nanoparticles from industrial processes. Wang and Kasper (1991), however, argued that 2–3 nanometer particles may penetrate the filter by bouncing off the filter internal surfaces. If this controversial prediction is true, it could mean a serious problem.

To investigate the possibility of such bounce in more detail, the researchers used molecular dynamics (MD) simulations that track the motion of the particle and surface atoms by integrating their equations of motion. The simulations sought to solve the above controversy by providing detailed collision information, which is difficult to obtain using other approaches.

Another aspect of the group's work concerned the collisions of nanoparticles with surfaces. This research bears on many applications, including material synthesis, microcontamination, and health effects. The properties of nanoparticles were expected to be different from those of large particles (e.g., micrometer range) due to the size effects or high proportion of atoms exposed to the surface. Accordingly, the interaction of nanoparticles with surfaces should be understood considering such effects. Classical MD methods were used in this study to understand particle-surface collisions from a microscopic viewpoint.

The main part of this project studied collision dynamics as a function of the incident velocity of particles. Materials of particles and surfaces were chosen so that they could simulate actual situations in filtration processes. The simulations in the research, which comprised the main part of this study, used computationally-intensive classical MD methods.

Visualization of particle trajectories is important both for understanding collision dynamics and presenting the results. The use of supercomputers, with algorithms suitable for multiple processors, dramatically reduced the com-

putation time of the simulation; specifically, the resources of the Basic Sciences Computing Laboratory were used to help in this visualization process.

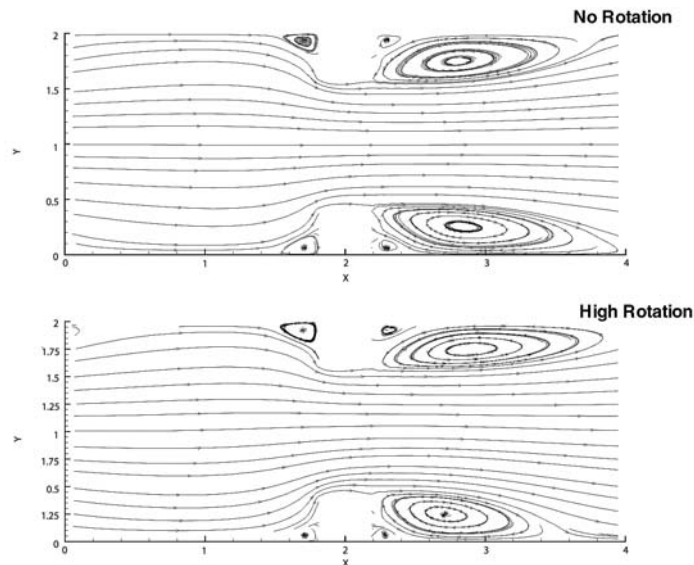
The researchers deposited particles in a tube with an abrupt contraction at low pressure. Prior to this, deposition mechanics such as this had been studied both experimentally and numerically: the main consideration of deposition mechanism here was the inertial impaction. In the experiment, the particle deposition efficiencies onto an orifice plate (orifice diameter: 1.16 cm) placed in a tube (inner diameter: 3.48 cm) were measured. The system pressure was controlled in a narrow range from 0.2 to 0.28 torr and the flow Reynolds number for the tube was 3.0. Spatially uniform aerosols were produced at low pressure by the method developed by Sato et al. (2000). The observed deposition curve, as a function of the particle Stokes number, was shown to be different from that obtained at atmospheric pressure for a Reynolds number greater than 1,000 (Chen and Pui, 1995). The difference was further confirmed by the numerical results for the cases with a Reynolds number of 3.0. The simulation also showed that the deposition curve had shifted to a smaller Stokes number as the Reynolds number increases. Empirical expressions for the deposition efficiency as a function of the Stokes number, the Reynolds number, and the contraction ratio (the ratio of the tube inner diameter to the orifice diameter), R , were given in order to estimate the particle deposition efficiency for any combination of these parameters for future applications. ■

Research Group and Collaborator

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Simulations of Flow and Heat Transfer in Complex Engineered Systems



Effect of rotation on the streamline pattern for turbulent flow through a ribbed channel.

These researchers considered 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 comparing predictions with grid-independent solutions. The second sought to evaluate the accuracy of RANS and subgrid turbulence models by comparing predicted results with experimentally measured ones. Spatially resolved experimental data on mean variables in inlets are available from the 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.

Furthermore, the following simulations were begun: RANS simulations of steady and unsteady flow in an axisymmetric mixed-compression inlet at different angles of attack, RANS simulation of flow in a gas-turbine cascade with contoured endwalls with and without film cooling, and LES of the intake flow in an axisymmetric piston engine with a centrally located valve.

A further area of study by this group focused on the LES of turbulent flow and heat transfer in propulsion systems. This work dealt in particular with flows in heat transfer and those containing separated regions. In the large eddy approach to simulating turbulent flow, empirical modeling was used only to represent effects of scales smaller than the computational grid. This approach showed much promise, but it is computationally intensive. However, the researchers believed that the time was right for increased research in this technique as more and more practical flow conditions came within reach of current and planned computers.

Some of the recent LES studies performed include the simulation of flow in a ribbed channel with heat transfer and rotation, the simulation of laminarization phenomena due to high heating in pipe flow, a study of the effects of buoyancy on turbulent structures, and the simulation of a rearward facing step flow with heat transfer.

The long-term goal of the research is to contribute to the physical understanding of cooling flows and transitional flows in propulsion sys-

tems. Comparisons are being made with the extensive experimental measurements made by the principal investigator's research group.

This research was computationally ambitious. However, it is important to bring the latest computational technology to bear on the most urgent problems that are limiting the competitiveness of the U.S. aeropropulsion industry in the global market. ■

Research Group and Collaborators

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Kumar K. Tamma, Fellow

Applications of Supercomputing to Interdisciplinary Computational Mechanics

This research constituted an effort toward the development of unified computational methodologies, solution algorithms, and finite element modeling/analysis strategies for interdisciplinary flow-thermal-structural problems. The philosophy and rationale advocated in the study was based on employing a common numerical methodology for each of the individual disciplines in conjunction with common computational algorithms for applicability to supercomputing systems in solving large-scale engineering problems. Various research activities included:

- Development of new time integration algorithms for transient problems
- Development of effective finite element based methodologies, which can be used in multi-disciplinary problems
- New physically correct contact models for penetration and impact problems
- Application of finite element methods in the manufacturing simulations
- Providing a paradigm for Virtual Manufacturing

The application areas included a wide range of engineering applications involving metal forming, casting, thermal degradation, and composite material processing. The overall efforts focused attention on providing new and effective approaches, for not only improving the existing applicability to supercomputing environments, but also toward providing an accurate understanding of the physics and mechanics relevant to multi-disciplinary engineering problems. ■

Research Group and Collaborator

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Michael R. Zachariah, Principal Investigator

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

These researchers worked in the area of high temperature chemistry and physics of vapor phase nanoparticle growth and microcombustion processes. Their studies were 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. The application sought the formation of new materials and the control of the emission of toxic heavy metal particles from combustors. The studies employed two theoretical approaches:

- Classical Molecular Dynamics (MD) simulations to understand particle-particle interactions and properties; specifically, these studies are aimed at determining particle-particle reactivity and physical/chemical properties of small particles (surface tension, internal pressure, etc.); in addition, faster algorithms for accelerating the MD computations were developed
- The CHEMKIN suite of programs used in the simulation of combustion and chemical vapor deposition processes

Ab initio molecular orbital methods were used to construct thermochemical databases and reaction rate data for the construction and testing of reaction mechanisms for reacting flows; the primary tool employed was the GUASSIAN suite of programs. The results from the MD and *ab initio* computations were used to feed reacting flow simulation programs aimed at simulating particle forming flows.

In one project, simulated nanoparticle formation was driven by chemical nucleation processes by incorporating aerosol dynamics models into the CHEMKIN software. In other studies, the group developed a MicroElectrical Mechanical Systems (MEMS)-based microcombustor model for a free-piston micro-engine. These studies were performed with the intention of

simulating the combustion on the microscale with detailed chemistry (several thousand chemical reactions). ■

Research Group

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Charles E. Campbell, Associate Fellow

Simulations of Macromagnetic Structure and Simulations of Quantum Fluid Systems at Low Temperature

These researchers executed a program of simulations of condensed matter systems, particularly in the two very different areas of micromagnetic materials and of quantum fluids. The principal effort in the former was on the determination of magnetic microstructure of magnetic materials on the scale of 50 nanometers to 100 microns, which were also studied experimentally in the Physics Department's Magnetic Microscopy Center (MMC). Of most interest were the mechanisms for spontaneous magnetic reversal, the structure of domain walls, and the effect of temperature, anisotropy, shape, and disorder on the writing to and stability of systems such as the microscopically thin permalloy films that were simulated by the group. At a similar level of interest was the appearance of unique structures in nanoscale nickel particles. Simulations also produced a new understanding of possible magnetic structures in such particles in the size range 50 nm to one micron, which should be very important technologically; these particles were grown and studied in the MMC.

One unanticipated outcome of this group's results is that it appears that the Zeeman energy introduced by a pulsed magnetic field may decay into non-linear spin-waves, an effect suggested recently as one of the principal sources of energetic damping within grains. The small-diameter systems that they have simulated thus far are ideal test beds for this possibility, which is one of the outstanding problems in present micromagnetics. The researchers are running spatially resolved continuous wave (CW) simulations to learn the source of the modes that are spun off from the main ferromagnetic response due to the presence of minority domains. The simulations seem to show spin waves carrying away some of the energy. The group's next task is to characterize these modes quantitatively.

Concerning the other area of this computationally intensive research, the researchers' quantum fluids simulation projects include potentially ground-breaking research in two areas: the impact of ^3He (i.e., fermion isotopic impurities) on the (boson) superfluid phase transition in liquid ^4He and the development of time-resolved quantum Monte Carlo simulations at finite temperatures. With regard to the former, the very low miscibility of ^3He in liquid ^4He requires very large simulation sizes, while the infamous sign problem in quantum Monte Carlo simulations of fermion systems requires the development of highly accurate importance sampling functions to successfully complete these simulations.

A related area of study for these researchers was identical particle scattering from a weakly coupled Bose condensed gas. Calculations were made of the scattering states and cross sections for a Bose condensed dilute gas trapped in a spherical square well of finite depth. The interactions were then treated in the scattering length approximation. The Gross-Pitaevskii and Bogoliubov equations for bound and scattering states were solved. The results indicated that there are transparency effects reminiscent of those conjectured to occur for strongly coupled systems. When incident particle wavelengths λ are comparable to the well size α , exchange-induced transparency enhancement is only dramatic for particular combinations of well depth, inter-action strength and particle number. For particles with large momenta ($\alpha/\lambda \gg 1$), however, exchange with the condensate results in enhanced transmission for all coupling strengths. Calculating the rate of decay of the scattering states to leading order in anharmonic corrections to the Bogoliubov approximation, the researchers found the corresponding inelastic cross sections to be extremely small. ■

Research Group and Collaborators

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Ming Yan, Graduate Student Researcher

Robert Zillich, Department of Chemistry, University of
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Cynthia A. Cattell, Associate Fellow

Studies of the Kinetic Physics of Planetary Magnetospheres

This research group examined 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 magnetotails of the Earth and Neptune. 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. Preliminary investigations of the stability of plasma distributions for four events strongly suggest that Electrostatic Ion Cyclotron waves observed by the satellite are caused by electron flow (either up or down the field line) rather than the concurrently observed ion flow. Recent work provided illumination on the relationship between cold and hot plasma modes, particularly the relationship to the transition between electrostatic and electromagnetic modes. Continuing investigation of FAST data focused on:

- Modeling further upward 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
- Simultaneous excitation of whistlers and solitary waves

This research's findings showed that an E/B ratio near c (the speed of light) does not imply that the electric field, E , is perpendicular to the wave vector, $\mathbf{k}$, or even that the dominant component of $\mathbf{E}$ is perpendicular to $\mathbf{k}$. This is contrary to the usual assumptions made in the interpretation of wave data. It was also shown that the electrostatic dispersion relation is accurate even when $E/B \sim c$, and that the magnetic

component of the wave can be predicted by using the electrostatic dispersion solutions in important terms in the electromagnetic dispersion tensor.

The researchers continued their study of the effects of electromagnetic fields, which occur on various spatial and temporal scales in the Earth's magnetotail, on the trajectories of particles to determine whether the phase space structures observed when there are no perturbations are substantially modified. This knowledge is critical to the understanding of the dynamics of the magnetosphere.

Supercomputing resources were used to examine the average energy changes and pitch angle changes to obtain an effective pitch angle diffusion coefficient. The researchers also produced distributions obtained using the more realistic wave fields (determined from experimental work) to compare the experimental observations. The numerical work involved modification of an existing code to model the plasma sheet boundary and the nonlinear electric field structures, which occur there based on the recently completely experimental studies of these structures. In addition, initial results indicated that these results may be partially influenced by the choice of global field model used. This result was then quantified statistically, to be used in future work.

These researchers also worked to describe how particle in cell simulations of solitary waves were performed using a 2D3V code with one electron and two ion species. Data from the FAST and Polar spacecraft are used to provide input parameters, and based on the observations no cold plasma was included in contrast to earlier simulations. Simulations containing both oxygen and hydrogen beams were compared to simulations that contain only hydrogen to examine the effects of the oxygen on the behavior of the solitary waves. In both cases, the solitary wave speeds were less than the hydrogen beam speed, and they were also

greater than the oxygen beam speed for the cases including oxygen. The simulated solitary waves had spatial scales on the order of $10\lambda_D$. These speeds and scale sizes were consistent with Polar spacecraft observations in the low altitude auroral zone.

In addition, the researchers considered solitary waves with large electric fields (up to 100 mV/m), which have been observed by the Polar spacecraft in the low altitude auroral zone and, at high altitude ($\sim 4\text{--}8\text{ RE}$, where RE equals the radius of the earth), during crossings of the plasma sheet boundary and cusp. Electron solitary waves are ubiquitous, and are observed for wide range of f_{ce}/f_{pe} . In contrast, to date, ion solitary waves have only been observed in the auroral zone at low altitudes in the region where $f_{ce}/f_{pe} \gg 1$. This work described some results of statistical studies of ion solitary waves at low altitudes and electron solitary waves at high altitudes. Ion solitary waves, observed in regions of upward field-aligned currents and ion beams, are negative potential structures and have velocities between O^+ and H^+ beam speeds, scale sizes of approximately $10\lambda_D$, and normalized amplitudes, $e\phi/kT_e$, of order 0.1 because the electron temperatures are large (plasma sheet values). In addition, the amplitude increased with both the velocity and the scale size, which is inconsistent with the predictions of ion acoustic soliton theory. The observations were well modeled by the simulations of Crumley et al. (2000), which included only the plasma sheet electrons and the beam ions. Both observations and the simulations were consistent with an ion hole mode associated with the ion two-stream instability. The high altitude electron solitary waves had velocities from $\sim 1,000\text{ km/s}$ to $> 2,500\text{ km/s}$. Observed scale sizes are on the order of $1\text{--}10\lambda_D$ with $e\phi/kT_e$ up to 0(1). For these solitary waves also, the amplitude increases with both the velocity and the scale size, consistent with electron hole modes, as was observed at low altitudes. Even

the very large amplitude solitary waves are stable based on the criterion developed by Muschietti et al. (1999).

This work also studied the results of ion trajectories traced through the T96 Tsyganenko magnetic field model with the inclusion of a perturbation electric field based upon satellite observations of lower hybrid waves in the magnetotail, as well as a simple convection electric field. The addition of waves with realistic parameters had a large impact on particle energies and steady state distribution functions for all regions of the plasma sheet and at all radial distances.

Finally, the researchers examined the use of kinetic simulations to trace particles through the magnetotail. These results offered a steady state particle tracing simulation using three different global magnetic field models, the Tsyganenko 1987, 1989, and 1996 models. Using distribution functions and their moments for all three models, the group compared and contrasted the various models with each other, with satellite data, and with other simulations to ascertain which features of the particle distributions are model dependent. They also showed the accuracy of each model in predicting particle distributions and their moments, showing that the choice of magnetic field model greatly impacts simulation results and can, if not careful, impact simulation interpretations.

Comparing the simulation distribution functions with satellite observations suggested that using this code with the T96 model gives results that fit data observations better than either the T87 or T89 model. ■

Research Group and Collaborators

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Study of the Geometric and Mechanical Properties of Molecular Gear Compounds

This research group is involved with the study of the geometric and mechanical properties of molecular gear compounds. They have investigated triptycene analogs on silicon surfaces using the GAUSSIAN computation package for electronic structure calculations. ■

Research Group

Shimin Hou, Research Associate

Alexander Grosberg, Fellow

Monte Carlo Simulations of Toy Proteins with Several Distinct Stable States; Computer Simulations of Cooperative Behavior of Biopolymers

Understanding how proteins self-assemble (“protein folding”) is a great challenge of modern molecular biophysics. Protein folding is traditionally associated with the self-organization of a unique native state of a heteropolymer molecule.

Real proteins must also have the ability to change their conformations in response to certain functional stimuli. In order to capture this effect in the framework of a minimalistic lattice model, this research group modified the sequence design method in such a way as to allow encoding of more than one stable conformation in the toy protein sequence. The dynamics of a polymer designed in this fashion are intimately related to the topology of its space of conformations. The researchers examined the relation between the broken ergodicity of conformational movements upon volume restrictions and the kinetics of conversion between different imprinted compact states.

Simulations of toy protein designs having more than one stable state are extremely computationally demanding due to exponential growth of intermediate states to be used.

The research group has tested its design algorithm on toy protein chains of 18 monomer links on a cubic lattice. This algorithm allows one to design a direct pathway of the rearrangement of the compact conformation on the cubic lattice. The main idea of this pathway design is based on the imprinting of the set of subsequently switching elements into the target conformation. The research group modified the sequence design method to encode energetic profile of the created conformational pathway. The fusion of the conformation and sequence design methods yielded a model protein with the entire one-dimensional sequence of stable conformations. The next challenge is to modify this approach for off-lattice models

of heteropolymers, which may shed light on the functionality of real protein molecules.

Another project by this research group involved charge inversion, which 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. This group’s successful molecular dynamics simulations are now being extended to include more realistic models, such as several of the macroions in the simulation domain and increased the volume fraction of surrounding solvent molecules closer to its realistic values. This is important to get closer to the practical question arising in the field of gene delivery. ■

Research Group and Collaborator

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Numerical Studies of Fluids and Disordered Solids

This group studied a variety of systems including the electrode-electrolyte interface, amorphous polymers, superfluid helium, and Bose-Einstein condensates using molecular dynamics. They used electronic structure methods—both separately and together in direct dynamics methods—for the former two, and quantum Monte Carlo and field theoretic models to study the latter. 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 were 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 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 Halley group elucidated the mechanism of ion transport in one of the prototype electrolytes. This led to new directions in the search for better ion conducting polymers at Lawrence Berkeley Laboratory, which recently produced very promising new polymer materials for this application. The polymer simulations, which use classical molecular dynamics at the atomic scale, are connected to longer time scales than are accessible by the traditional methods by a variety of techniques, some of them developed in this group, including a form of renormalized molecular dynamics and an innovative application of the parallel replica method.

The work on Bose-Einstein condensates was motivated by a search for better experimental probes of the condensate, particularly in liquid helium four. To evaluate a proposal by this group for a new kind of helium atom scattering experiment to study the condensate, they carried out both strong coupling variational calculations and weak coupling calculations at the Bogoliubov level. Helium is a strongly coupled fluid, but the weak coupling calculations permit evaluation of the validity of the strong coupling results, because they involve approximations that are better controlled. Also, weak coupling calculations apply directly to a newly discovered set of Bose-condensed alkali gases. The results of recent weak coupling calculations showed that there are transparency effects reminiscent of those conjectured to occur for strongly coupled systems.

In another category of calculations associated with the condensate studies, members of the group simulated the behavior of pulsed atomic helium beams, which are used in the experiment to study the condensate in liquid helium four. Using a gas dynamics code to model

these pulsed low energy helium beams, the workers found a good fit with the experimental results at low source power. The fit implied that significant collisional effects occur in these beams. The code could also be used to simulate signals to be expected in the experiment (not yet carried out) in which the beams will be used to study the condensate in liquid helium four. Very recently, these gas dynamics codes were used in a computationally innovative way to predict the behavior of atomic helium pulses of much higher density, which behave anomalously in the experiments. To simulate these pulses in which millions of atoms are involved, the group (in particular, Aaron Wynveen) wrote a hybrid code in which the molecular dynamics portion was used to determine a boundary condition for the continuum hydrodynamic description of the gas used in most of the volume of the simulated space. This simulation recently produced results quite similar to the anomalous experimental results and suggests an explanation in terms of shock waves in the pulse. ■

Research Group and Collaborators

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Data Analysis of Cosmic Microwave Background Experiments; Model Robust Designs

These researchers continued to analyze and estimate cosmological parameters from the data collected by the MAXIMA-1 and MAXIMA-2 balloon-borne experiments. The data constrained several of the parameters that determine the evolution of the universe. Using both the Bayesian and frequentist statistical approaches in the analysis, the researchers compared the values obtained in each. In general, they achieved substantial progress and expected further advances in the research period to come.

The research group has also begun a project to design and test the data analysis pipeline that will be used to analyze the forthcoming MAXIPOL data set. MAXIPOL is a balloon-borne experiment that will search for polarization in the cosmic microwave background (CMB). Also, we will continue to build on our existing software used to determine cosmological parameters from measurements of temperature anisotropy of the CMB.

Another new area of research for this group includes development of an algorithmic approach to the construction of a class of model robust designs including supersaturated designs and response-surface design. Combined with other related work in computer-aided algorithms, the research will fundamentally change the way of selecting experimental designs in both academia and industry, i.e. shifting from traditional approaches that rely on design tables to algorithmic approaches that can better address the flexibility and design efficiency in today's world. Model-robust designs usually consider many different possible models that can increase exponentially with the run size and are therefore very computationally intensive, requiring the resources of the Supercomputing Institute. ■

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Analysis of Nuclear Reaction Data

During the late eighties and early nineties, a number of experiments were performed at Los Alamos Meson Physics Facility and at the Indiana University Cyclotron. These consisted of proton scattering and two-neutron pickup reactions. The purpose was to investigate the basic nucleon-nucleon (NN) interaction inside the nucleus, which differs from the free NN interaction. There are several controversial and somewhat conflicting theories of how the free NN interaction is modified by the presence of other nucleons. Fundamentally, the underlying quark structure of neutrons and protons (nucleons) is involved. Analysis of the data requires numerical integration of second-order partial differential equations in three dimensions.

In most problems worked on by these researchers, sets of coupled differential equations were involved and many interactions are required in parameter search routines. This research group has begun to collaborate with a physicist at the University of Colorado to develop a more sophisticated program for analysis of the two particle transfer data. The results of this project were expected to have important implications in astrophysics, particle physics, and condensed matter physics. ■

Research Group

Michael A. Franey, Research Associate

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Numerical Investigations 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.

These 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 magnetohydrodynamic (MHD) code provided by the group lead by Thomas W. Jones of the Astronomy Department. The main focus in this area was on an investigation of the nonlinear dynamics of the magnetospheric tail using this code. In addition, the researchers continued their investigations of the Kelvin-Helmholtz instability and the excitation of field line resonances.

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. Having made the first steps in modifying the nonlinear MHD code described above to model the low- β plasma in the auroral acceleration region. The researchers also included the effects of neutral winds in their calculations.

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. This effort helped 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 Aeronautics and Space Administration (NASA) 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 hoped to more efficiently simulate these structures.

Specific projects, based on the implementation of the above research profile, included the MHD simulation of magnetospheric waveguide modes. Ultralow frequency waves with frequencies of 1.3, 1.9, 2.6, and 3.4 mHz are often observed and associated with field line resonances (FLRs) in the inner magnetosphere of the Earth. Waveguide modes were proposed as a mechanism for generating FLRs. Using a compressible two-dimensional MHD simulation, the researchers explored the nonlinear effects on the excitation of waveguide modes and frequencies of the modes. Changes in key parameters and how they affect waveguide modes were analyzed.

Another project developed by this group produced a three-dimensional model for the propagation of Alfvén waves through the auroral ionosphere. The propagation of Alfvén waves in the auroral ionosphere is important in the determination of ground signatures of time-varying currents, in the formation of Pc1 compressional waves that can be ducted in the ionosphere waveguide, and in the development of field-aligned currents and parallel electric fields

during auroral acceleration processes. This research presented the first results from a three-dimensional model of the linear propagation of these waves. In this model, the ionosphere was treated as a thin slab carrying Pedersen and Hall currents. The jump conditions across this boundary lead to the coupling of shear and compressional MHD modes at the ionosphere and also allowed the ground signatures of these waves to be calculated within the context of the model. This model was used to study the coupling and to illustrate the excitation and propagation of compressional MHD waves within the ionospheric waveguide. A new numerical scheme for the modeling of parallel electric fields was also introduced and the excitation of resonance cone structures by narrow impulses was then demonstrated.

These researchers also performed studies of ion solitary waves using simulations including hydrogen and oxygen beams. Particle in cell simulations of solitary waves have been performed using a 2D3V code with one electron and two ion species. Data from the FAST and Polar spacecraft are used to provide input parameters, and based on the observations no cold plasma was included in contrast to earlier simulations. Simulations containing both oxygen and hydrogen beams were compared to simulations that contain only hydrogen to examine the effects of the oxygen on the behavior of the solitary waves. In both cases, the solitary wave speeds are less than the hydrogen beam speed, and they are also greater than the oxygen beam speed for the cases including oxygen. The simulated solitary waves have spatial scales on the order of $10\lambda_D$. These speeds and scale sizes are consistent with Polar spacecraft observations in the low altitude auroral zone. ■

Research Group and Collaborators

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Oriol T. Valls, Fellow

Numerical Studies in Condensed Matter Theory

This group continued to enhance its ongoing research program in the following areas:

- Non-linear electrodynamic properties of unconventional superconductors
- Proximity effects at superconductor/ferromagnet interfaces and structures
- Phase diagram of glassy materials, particularly in layered vortex systems and hard spheres
- Phase diagram of the superconducting vortex system in the presence of pinning centers ■

Research Group and Collaborators

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University of Minnesota—Twin Cities

Medical School

Cancer Center

Stephen S. Hecht	217
------------------------	-----

Department of Laboratory Medicine and Pathology

Lynda B. M. Ellis	218
William B. Gleason	219
Franz Halberg and Germaine Cornélisson	220
Kristin A. Hogquist	222
Christopher Pennell	223

Department of Neuroscience

Bagrat Amirikian.....	224
Linda M. Boland.....	225
George L. Wilcox.....	226

Department of Orthopaedic Surgery

Jack L. Lewis.....	228
--------------------	-----

Department of Otolaryngology

Peter Santi.....	229
------------------	-----

Department of Pharmacology

Rodney L. Johnson.....	230
Stanley A. Thayer	231

Department of Physiology

Jürgen F. Fohlmeister	232
David Levitt	234

Department of Radiology

Rolf Gruetter	235
J. Thomas Vaughan	236

Department of Surgery

Kristin Gillingham	237
Lester Floyd Harris and Leonard S. Schultz.....	238
Carl S. Smith	240

Department of Therapeutic Radiology–Radiation Oncology

Dan Vallera	241
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Stephen S. Hecht, Principal Investigator

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

Cigarette smoking causes approximately 30% of all cancer deaths in the U.S. In spite of advances in tobacco control and smoking cessation, there are still 48 million smokers in the U.S., including about 25% of the adult population. Approximately 500 billion cigarettes and 121 million pounds of smokeless tobacco were consumed in 1997 in the U.S.

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-(methylnitrosamino)-1-(3-pyridyl)-1-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, on the extensive data on the occurrence of NNK and NNN in tobacco products, and on biochemical studies, these researchers hypothesized that such compounds play a significant role as causative factors in human cancers associated with tobacco use.

This research group's specific aims were 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 NNAL, determining differences in the stereoselectivity of metabolic activation of NNK, and examining differences in the metabolic activation and carcinogenicity of NNN enantiomers

- Deoxyribonucleic acid (DNA) and protein pyridyloxy-butylation by NNK and NNN by elucidating the structures of the major adducts formed with DNA and hemoglobin
- 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

The overall theme of this work was based on mechanistic studies of NNK and NNN metabolism and adduct formation, in order to further evaluate the carcinogenic potential of NNK and NNN in humans exposed to tobacco products. ■

Research Group

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Lynda B. M. Ellis, Principal Investigator

Predicting Structure of Proteins With Remote Sequence Similarities

This research group developed sequence-based methods to detect remote protein sequence similarities (homologies) that are or are not indicative of protein structural and functional similarities. The methods were developed, tested, and evaluated using non-redundant pair wise test sets that contain proteins of known sequence and structure. The researchers emphasized identifying sequence pairs that have similar sequence with dissimilar structure and those that have dissimilar sequence with similar structure. ■

Research Group

Edward Bryan, Research Associate

Paul Tavernier, Research Associate

Fei Xu, Research Associate

William B. Gleason, Fellow

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

Parallel processing strategies of potential widespread utility in mass spectrometry 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 small Linux clusters comprised of moderately-priced hardware, e.g. Pentium or AMD-based systems. 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 high performance computers with large memory and disk capabilities is attractive. The most recent version (1.0.8) of the free-available program *cIdentify* (a derivative of Pearson’s *FASTA* program) has been compiled and run using the message passing interface (MPI) so that it can be executed on multiple-processor hardware under the Linux operating system on the Supercomputing Institute’s IBM Netfinity cluster. Parallel versions, also MPI-based, have also been developed to run on other multi-processor computers, currently the Silicon Graphics Origin series and the IBM SP series.

This group is also studying the interaction of proteins with sulfated carbohydrate polymers related to the anticoagulant glycosaminoglycan, heparin. *Ab initio* calculations, using the *GAUSSIAN* package, are being used to develop suitable parameters for sulfated carbohydrates. Molecular dynamics (using Schulten’s *NAMD/VMD* package) simulations of sulfated model carbohydrates, including explicit solvent, are being used to test the parameterization. Schulten’s package is particularly useful because it scales very well when being used in parallel mode on multiple processors. In preparation for studying the interaction of sulfated materials with proteins, we have learned how to inter-

actively control ligand interactions with macromolecules while a simulation is in progress. Ultimately, this capability will allow us to perform simulations more efficiently. ■

Research Group and Collaborator

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William Ojala, Research Associate

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Germaine Cornélisson, Co-Principal Investigator

Chronobiologic Assessment of Physiologic Chronomes From Womb to Tomb

Strokes and other adverse vascular events are major crippers, costing the United States an estimated yearly cost of over \$30 billion. These researchers developed a system for the chronobiologic analysis of cardiovascular records with a focus on disease prevention. Ambulatory devices are now used in different geographic locations for the automatic monitoring of blood pressure and the electrocardiogram (ECG) for seven days at the outset. Chronobiologic analyses of such records serve first and foremost to improve screening, diagnosis, and treatment. From a basic viewpoint, they also serve to assess how environmental factors affect human physiology, notably heart rate, and blood pressure. The pursuit of these goals was greatly facilitated by access to the supercomputing resources, in order to:

- Analyze beat-to-beat records for resolving chronobiologic and chaotic endpoints (a typical record consists of about 2,400,000 data resampled as 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 on at-risk individuals longitudinally by means of control charts

A chronotherapeutic trial was also pursued to optimize the timing of treatment of blood pressure disorders.

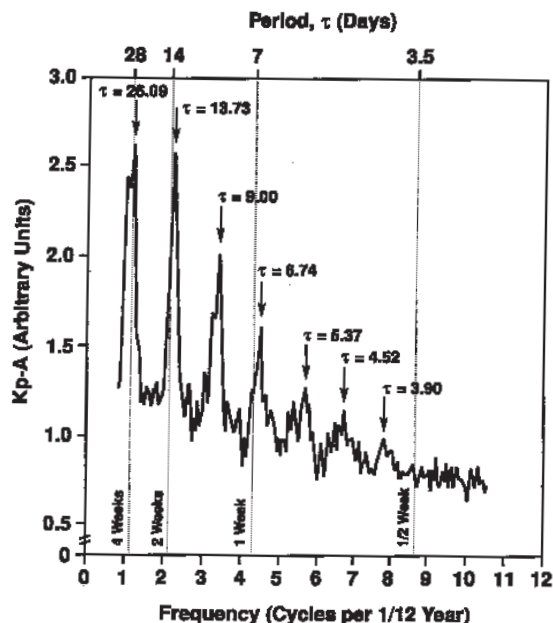
Toward this goal, several new programs were developed, and these and existing programs were routinely applied for data analysis as they accumulate. Existing records were organized into databases so that reference values could be regularly updated and any abnormality easily detected. A library of programs for such chronobiologic applications was organized and integrated with the incorporation of graphic displays of the results.

A reduced heart rate variability and an excessive circadian blood pressure amplitude (circadian hyper-amplitude-tension: CHAT) were identified as risk factors by these researchers, and have since been documented as largely independent, both contributing additively to the risk of adverse vascular events.

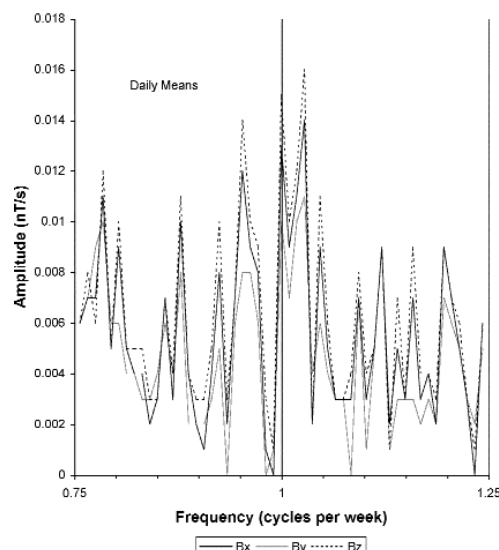
Environmental effects on heart rate variability and other aspects of human physiology are slowly being recognized, with new confirmation from seven-day ECG records obtained above the Arctic Circle. The phase relation within the solar activity cycle shows a sequence of events that makes physiological sense. Cross-spectral techniques relating the biological information to physical records (also available at short intervals for very long spans, some covering several hundred years) thus gain in interest from a basic viewpoint as well. ■

Collaborator

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Least-squares fit of harmonics, separately to 3-hourly values of each calendar year, using steps equal in frequency between 10 cycles/year and one cycle per 70 hours (A =average amplitude). The spectrum of the global planetary index of geomagnetic activity, K_p (index of disturbance of the horizontal component of the geomagnetic field), available at three-hour intervals for 59 years (1932–1990), reveals, with the approximately 27-day solar rotation component, a high harmonic content. This includes an approximately weekly component with a period of 6.74 days, a statistically-significant difference from exactly 7 days.



Partial spectra of data from a stand-alone magnetometer residing within the British Antarctic Survey Automated Geophysical Observatory A80. The records represent geomagnetic pulsations sampled at 0.5-second intervals from Jan. 1, 1997 to Jan 31, 1999, in an isolated area 600 km from the nearest human habitation. The three spectra correspond to the three coordinates of dB/dt (in nT/s). They were obtained on the daily mean values of 1-min standard deviations of the original 0.5-second data, analyzed over a 25-month span. Two distinct spectral peaks are observed, corresponding to signals validated by nonlinear least squares, one with a period of exactly 7 days, the other—slightly more prominent—with a period of about 6.8 days, similar to that characterizing K_p . Whereas the latter likely represents the natural component, the former may be indicative of human pollution. Components of approximately seven days are often encountered in biology. Their period was found to be inherited in studies of twin neonates by intra-class correlation analyses. This biological week is important for the patterning in time of treatment, as shown already in the case of cancer chronotherapy

Kristin A. Hogquist, Principal Investigator

Peptide Introduction of Positive Selection

Positive and negative selection are the critical forces that shape the T cell repertoire. These researchers addressed 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. Using confocal microscopy and gene array technology, the researchers attempted to identify the molecules integral to the processes of positive and negative selection of T lymphocytes. ■

Research Group

Timothy Starr, Graduate Student Researcher

Christopher Pennell, Principal Investigator

Human RNase in Immunotoxins

An immunotoxin is a two-component construct designed to target and kill a particular cell type. Historically, plant or bacterial toxins are used as the toxin component in their construction. A drawback to using plant or bacterial toxins is their inherent immunogenicity. An appealing alternative to plant or bacterial toxins are human ribonucleases (RNase). A limitation to the use of human RNases in an immunotoxin is their potent intracellular inhibition by ribonuclease inhibitor (RI).

This research group is analyzing the effect of specific mutations of human RNase in the context of their interaction with ribonuclease inhibitor. Mutations which appear to inhibit the interaction with RI will be performed with the goal of producing more potent, less immunogenic immunotoxins. ■

Research Group

Heidi Erickson, Research Associate

Bagrat Amirikian, Principal Investigator

Three-Dimensional Lattice Model of the Motor Cortex: Emergence of Topologically Ordered Neuronal Structures with Coherent Properties

The long-term goal of this research was 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 combining theoretical methods with experimental approaches. In this work, the researchers endeavored to advance the understanding of whether and how the spatio-structural constraints on intrinsic connectivity effect the segregation of neurons into functional modules. A three-dimensional lattice model, generated by this research, 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, which is heavily based on the accumulated knowledge of the neuroanatomy and neurophysiology of the motor cortex, lies at the root of the present attempt to bridge theoretical frameworks and experimental data in the domain of very large-scale simulations of networks of simplified neurons.

Two principal developments in science and technology made this project feasible: extension of quantitative studies of local cortical connectivity into the spatial domain, and emergence of high performance parallel supercomputers. ■

Research Group

Thomas Naselaris, Graduate Student Researcher

Linda M. Boland, Principal Investigator

Simulations of Voltage-Dependent Ion Channel Gating

Voltage-gated ion channels regulate the electrical properties of excitable cells. These researchers were interested in understanding the mechanisms of ion channel opening and closing, which alters cellular excitability and biological signaling. Continuous-time, discrete-state Markov models were used to reconstruct experimentally measured ionic and gating currents from ion channels. Numerical time-integration of mathematical models was performed using an implicit method with a variable-step, variable-order backward differentiation time-stepper, a Newton nonlinear solver, and an iterative linear solver with simple reconditioning. A novel, inexpensive computational method for the estimation of asymptotic and finite-time gating charge was used in the lab. Experimental data was compared with simulations in order to estimate optimal parameter values that reconstruct the electrophysiological experiments. Regression analyses were carried out in parallel to improve the ability to find a true global optimal set of model parameters. These simulations proved useful in evaluating current hypotheses about channel gating mechanisms, making predictions, and generating ideas for new experiments in the lab.

This project further refined several models of potassium ion channel gating. Potassium channel gating was modeled by classical kinetic theory with voltage-dependent rate constants and the assumption that gating is a Markov process. This research used models to simulate the modification of inactivation gating by accessory (non-pore-forming) protein subunits or the modification of activation gating by drugs or biomolecules. Animated graphical outputs of the channel's behavior under different experimental conditions were generated and compared to experimental data generated in ongoing electrophysiological and structure-function experiments. This process was expected to use

a heuristic search for the most sensitive model parameters, which, in turn, were to be used as starting points for multiple nonlinear regression searches in the remaining parameter space.

These researchers successfully developed three different models of potassium channel gating and applied these models to experimental data. The experimental data was simulated by the mathematical calculations of the model using user-defined criteria. The greatest challenge was selecting the best fit parameters. Since this was not achievable by trial and error, the research group continued to work on fitting the free parameters in the simulation using methods for error minimization. Supercomputer resources were critical to the development and testing of methods to search for the best fit parameter values. ■

Research Group

Anthony Varghese, Research Associate

George L. Wilcox, Fellow

Axonal Propagation of Impulses in Peripheral Afferents

This research team focused on the mechanisms of pain signaling and analgesia. Computational work in this lab involved the function of neurons of the central and peripheral systems and in particular the simulation of electrical excitability using data from new experimental techniques in molecular biology. An object-oriented approach to incorporating molecular information allowed the team to simulate phenotypes or the effects of genetic variations and mutations at the tissue level. The response of these cells to pharmaceutical interventions was also explored. A sound numerical time-integration scheme comprising a backward-differentiation time-stepper, a modified Newton nonlinear solver, and a preconditioned Krylov subspace iterative linear solver were used. The cells chosen for the initial part of this project are A- δ and C-fibers from rat dorsal root ganglia and rabbit cardiac sinoatrial node cells. These cells were chosen on the basis of molecular information available from the group's 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 enjoyed a wide range of applicability. They serve as a prototype for exploring disturbances 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. The use of mutation information allowed the researchers to examine various diseased states and the use of pharmaceutical agents allowed researchers to explore options in therapy in patient therapy.

This group is continuing a neuronal simulation project that was started in January 1998. A computational model of the geometry of myelination was constructed, and both implicit and explicit numerical time integrators were implemented and tested for parallel performance. The researchers continued to work on more

realistic ion channel mechanisms for the simulations performed by the group.

It should be noted that the group took a risk in using c++ as the language for this project. In the short term, this slowed progress, since support on the Origin 2000 for parallelization of c++ was not as extensive as it was for FORTRAN; in addition, changes to the operating systems resulted in the SP c++ compilers being unable to link to the FORTRAN modules thus slowing progress on the SP. Further, changes on the Origin 2000 resulted in previously parallel code being forced to run in serial mode; this resulted in very poor performance for some time on the Origin. A Kuck and Associates Inc. C++ compiler was tested by these researchers, using OpenMP parallelization directives; since this compiler uses native IBM SP compilers, IBM delivered an ANSI c++ compiler. This aided greatly in code development.

The researchers expected a benefit from the object-oriented features of c++ (based on recent upgrades of the models) as the ion channel mechanisms and their interactions with drugs are elucidated.

Feasibility studies regarding the computational requirements of the multidimensional audio-visualization project were undertaken and show promising results in the development of a novel method of display of large, multidimensional data sets. The infrastructure and custom software to be developed relied primarily on the FORTRAN 90 programming environment. The language can be made to run optimally in a parallel environment. C code may be used in conjunction to gain cross-compatibility with older custom software used for data analyses as well as for other computations. ■

Research Group and Collaborator

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Anthony Varghese, Research Associate

Jack L. Lewis, Principal Investigator

Biomechanics of Articular Cartilage

Articular cartilage weakens and fractures during the progression of osteoarthritis. The goal of this group's research is to understand disease processes and matrix assembly processes for cartilage. Cartilage weakens in disease, but the underlying cause is usually unknown. The strength of artificial cartilage, as a replacement for diseased cartilage, is not yet as high as that of natural cartilage.

The strategy to address both of these issues is to understand the relationship between cartilage strength and microstructure. This group is developing test methods for measuring the failure properties of cartilage and other soft tissues, using stress analysis of candidate test specimens as one tool. They are also developing microstructural models that simulate cartilage microstructural composition and morphology. These models are analyzed using finite element analysis or other analytical methods, and related to macroscopic material properties. The numerical work parallels experiments designed to analyze and characterize articular cartilage and its microstructure. ■

Research Group

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Se-ho Park, Graduate Student Researcher

Peter Santi, Principal Investigator

Computer Image Analysis and Three-Dimensional Reconstruction of the Mouse Cochlea

Research Group

Vladimir L. Tsuprun, Research Associate

The mammalian cochlea contains a complex array of specialized cells and tissues that are required for normal hearing. Although their morphology is well known, their molecular anatomy is poorly understood. This research group's goal is to provide a detailed understanding of the structure and function of the glycoconjugate components of the extracellular matrix of the cochlea in order to better understand normal hearing and the basis of certain hearing dysfunctions. Using immunohistochemistry they have provided a number of "first descriptions" of important glycoconjugate components of the cochlea. However, the composition of other cochlear glycoconjugates is unknown and has only been revealed by non-immunological methods. These macromolecules have unique structures and occupy critical sites within the cochlea that are important in fluid transport and hair cell transduction.

During the last year this group has characterized the size, shape, charge, and distribution of glycoconjugates of the four different types of basement membranes. In another study, they have described a triple helical arrangement of unknown glycoconjugate macromolecules that constitute the mechanoelectrical strand of the hair cell. These structures are called tip-links, and together with the side and attachments links, they provide a framework for transduction of sound-induced mechanical energy into receptor potential changes and ultimately as hearing. For the coming year, the group has adopted the mouse as their animal model due to the wealth of genomic information being generated for this species. They also plan to use three-dimensional reconstruction methods to analyze the macromolecular relationships between these complex, space-filling glycoconjugate components. ■

Rodney L. Johnson, Principal Investigator

Design and Synthesis of Blocker q Human 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. Recent modeling studies have been conducted with scorpion toxins, known blockers of KV1.3, with inhibition on the pico to nanomolar range. Based on this work, this research group has established a model of KV1.3. Using this model as a reference, potent and selective small molecule blockers of KV1.3 could be developed. ■

Research Group

Abigail Fisher, Graduate Student Researcher

Ashish Vartak, Graduate Student Researcher

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. Over-stimulation of glutamate receptors results in Ca^{2+} overloading and mitochondrial dysfunction. These researchers are investigating whether the interactions between Ca^{2+} and mitochondria contribute to glutamate-induced neurotoxicity. Varieties of techniques were employed to examine the intraneuronal and intramitochondrial Ca^{2+} concentrations, neuronal viability, mitochondrial function and molecular events triggered by mitochondrial uptake of Ca^{2+} . Pharmacological agents and molecular engineering approaches were used to dissect the molecular pathways involved, and to identify the targets for intervention. ■

Research Group

Guang Wang, Research Associate

Jürgen F. Fohlmeister, Principal Investigator

Computational Neuroscience

This research project involves the simultaneous solution of 9 to 14 non-linear differential equations for the purpose of determining the parameters of rate constants for the gating of 5 or 6 ionic channels. Furthermore, the channels were distributed non-uniformly throughout the complex geometry of the neuron membrane. The effects of this geometry on the encoding of nerve impulses were then evaluated.

This group also investigated the role of membrane capacitance in neural excitation. Although membrane capacitance ($1 \mu\text{F}/\text{cm}^2$) was accurately measured about two decades prior to the first delineation of the ionic current responsible for the nerve impulse (the Hodgkin-Huxley model), capacitance of neural membrane has generally been regarded as an unavoidable and unimportant linear current path in parallel with the critical sodium, calcium, and potassium 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 group 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 has the important function of determining the scale for the magnitude of the ionic current necessary for impulse generation. In the non-space-clamped neuron, specifically in neurons with non-uniform channel density distributions, the capacitance can act as a battery in that stimulus current can charge the membrane capacitance, which is capable of holding its voltage under certain circumstances. This occurs when regions of low channel density are present in the neural morphology; the locally low charge leakage can control the dynamic range of impulse frequency genera-

tion. 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 electrically gated channel densities, also interact with their neighboring membranes to determine rate of impulse firing.

This group also studied the Hodgkin-Huxley model equations. 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 (1952) equations have 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. The researchers have discovered 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 3 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 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 (large dV/dt) of the Na-current is compromised by the necessarily accompanying large capacitative current, which is proportional to dV/dt ; the slower recovering K-current is associated with

a smaller time-rate of voltage change (dV/dt) and is therefore less affected by capacitative current. It is shown that phase space analysis offers the necessary adjustments to voltage-clamp data, which are typically contaminated 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.

A final area of research involved creating a model, called the “sticky model,” which simulates the primordial accreting process of continents and their associated tectonic plates. Buoyant “flakes” of hard material 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. The cells (Rayleigh-Benard convection) are defined by Voronoi polygons based on the distributed hotspots. The Voronoi edges represent convective down-welling regions, among which certain Voronoi triple junctions act as nucleation points for the accumulation of the buoyant material (flakes), which does not descend with the bulk mantle material. The accumulation represents the growth of the primordial continents, and associated tectonic plates. While flakes are moving, the nascent plates independently undergo rigid body motion imposed by the viscous shear forces exerted by the underlying convecting mantle. When a flake touches a plate it sticks to that plate and becomes a part of that plate, thus increasing the plate area. Tiny, aboriginal plates can be of arbitrary shape; their areas however grow much more rapidly along the Voronoi edges than elsewhere by the present model accretion process, resulting in star-shaped proto-continents. When the plate area has grown to encroach upon, and cover the hotspots, the plate rotates erratically and begins to move away from its nucleation point, to

wander over the global surface driven by the mantle convection cells. Plate-to-plate collisions occur, resulting in supercontinents, and the classical Wilson cycle of the accretion of supercontinents and their breakup will have begun. ■

David Levitt, Principal Investigator

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 (SMAD) phasing techniques made the generation of high-resolution electron density maps a routine procedure; the researchers began developing a program to automate this. The goal was to submit the electron density map and the amino acid sequence to the computer, which then returns an accurate initial structure that can be used as input to refinement programs. These researchers found they were able to automatically fit nearly all secondary structures. The next step was to extend secondary structures into the loop regions.

The researchers also performed routine refinement of x-ray crystallographic protein structures using either XPLOR and NCS. Testing was undertaken for a new software package under development; this attempted to automate the fitting of electron density maps. It should be possible to assign the amino acid residues, complete the loops, and refine the side chain atom positions.

The development of these programs required extensive time on a graphics workstation. Each step in the fitting process was monitored using a protein visualization program developed specifically for this project. In addition, a large number of procedures required optimization. The most direct way was to run the program many times with different parameter sets and find the set that gives the best fit to the density. This optimization was performed on the Origin 2000. ■

Research Group

Mariah B. Olson, Supercomputing Institute Undergraduate Intern

Rolf Gruetter, Principal Investigator

Analyzing Spectra Using One-Dimensional and Two-Dimensional Methods

This research group focused on analyzing spectra using one-dimensional and two-dimensional methods applied using the high-resolution nuclear magnetic resonance (NMR) facility and *in vivo* data. Specifically, the group is focused on detailing the information content of such spectra, spectral simulations, and the fitting of systems of 25 different equations to time courses measured *in vivo*.

The research group is working 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.

To this end, the group will:

- Pinpoint the modeling constraints that are necessary to determine the rate of neurotransmission in the brain *in vivo*
- Measure approximately 20 neurochemicals simultaneously *in vivo* from very small volumes ■

Research Group

Gulin Oz, Graduate Student Researcher

Ivan Tkac, Research Associate

J. Thomas Vaughan, Principal Investigator

Simulation of High Frequency RF Volume Coils

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. But as frequency increases, radiation losses rise dramatically, affecting the efficiency of the coils and causing the imaging quality to deteriorate. This research group is using computer modeling to simulate the high-frequency RF volume coils in order to study how these problems can be avoided. ■

Research Group

Jinfeng Tian, Graduate Student Researcher

Kristin Gillingham, Principal Investigator

Random Assignment of Treatments in Solid Organ Transplant Research

In solid organ transplant research, many randomized clinical trials are conducted. The researchers wrote a program in FORTRAN 77 that allowed them to carry out the random assignment of various treatments to their study patients. In the past, this randomization program was run on the University's NOS computer system. After this system was shut down, the researchers used Supercomputing Institute resources in order to access the International Mathematical and Statistical Library and to implement their randomization program. ■

Research Group

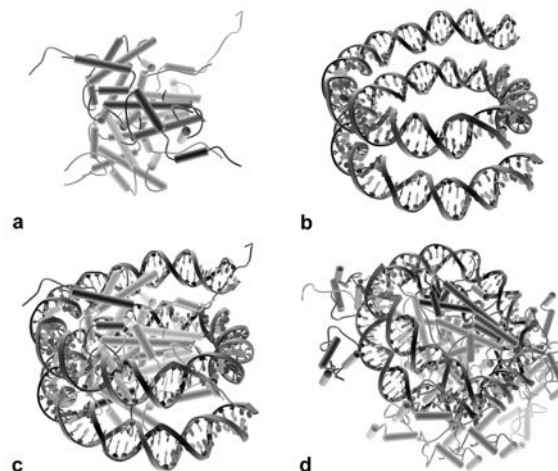
Yan Zheng, Staff

Lester Floyd Harris, Principal Investigator Leonard S. Schultz, Co-Principal Investigator

Dynamic Simulations of Solvated Protein/DNA Complexes

These researchers conducted experiments investigating the mechanism(s) of a genetic switch controlled by deoxyribonucleic acid (DNA) regulatory proteins. Interest lay in steroid hormone receptor protein interaction with DNA in the pathogenesis of breast cancer. The researchers previously reported on a mechanism describing how these DNA regulatory proteins recognize and bind to their specific sites on DNA. In the most recent research period, they conducted molecular dynamics simulations in solvent to investigate hydrogen bonding, van der Waals and electrostatic interactions between amino acids of the DNA regulatory proteins, and nucleotides of their cognate DNA binding sites. They used a biological model of a virus that infects bacteria, a bacteriophage, for investigating the genetic switch controlling lytic/lysogeny expression in the 434 bacteriophage. It is known that this genetic switch is under the control of two proteins of the bacteriophage, cI repressor and Cro, that interact with DNA sites, operators OR1, OR2, and OR3, within the bacteriophage genome. The cI repressor protein preferentially binds first to OR1 then to OR2 inducing transcription to the left. In contrast, the Cro protein preferentially binds first to OR3 then OR2 inducing transcription to the right. The basic molecular interactions between amino acids from the bacteriophage proteins interacting with specific regulatory sites on DNA are in agreement with the researchers' earlier findings for the amino acids of the steroid hormone receptor proteins interacting with their regulatory sites on DNA. Together these findings strongly support their theory that proteins recognize specific sites on DNA based on stereochemical complementarity and conservation of genetic information between the proteins and the specific sites on DNA to which they bind and turn genes off or on.

While bacteriophage genome, lacking a nucleus and chromosomes, is very simple in its



Computer models of the mouse mammary tumor virus (MMTV) nucleosome structure and its components: *a*) the histone core is made up of an octamer composed of two each of histone proteins H2A, H2B, H3, and H4; *b*) 146 base pair MMTV LTR DNA wrapped in a superhelical conformation; *c*) the superhelical DNA wrapped around the histone protein octamer core; *d*) the MMTV nucleosome with five glucocorticoid receptor proteins docked at their response element DNA sequences.

organization and structure, the genome of higher forms of life is very organized, compact, and structurally complex, and contains a nucleus and chromosomes. The DNA of the chromosomes is packaged in a complex structure, chromatin, with the aid of specialized proteins called histones. The fundamental packing unit of the chromatin is the nucleosome, which is conserved, in all higher forms of life. The nucleosome consists of 146 nucleotide base pairs wrapped around a histone core (see figure, parts *a–c*). The histone core is made up of an octamer composed of two each of histones: H2A, H2B, H3, and H4 (see part *a* of figure). Recently, a nucleosome structure has been crystallized and its atomic co-ordinates have been determined by x-ray crystallography. These researchers used these atomic coordinates as a template to construct a nucleosome

model of the 146 base pair DNA sequence of the long terminal repeat, LTR, flanking the mouse mammary tumor virus genome that is rich in binding sites for steroid hormone receptor proteins. This LTR DNA sequence contains five specific DNA binding sites, glucocorticoid response elements (GREs), for the glucocorticoid receptor protein that is involved in genetic regulation of the mouse mammary tumor virus genome. These researchers use the mouse mammary tumor virus as a model for studying steroid hormone regulation of genes in breast cancer. As seen with the bacteriophage operator DNA sequence of the genetic switch, the GREs within the LTR DNA sequence function in concert to regulate the mouse mammary tumor virus genome. Earlier, these researchers conducted molecular dynamics simulations on one of the five GREs of the LTR as an extracted DNA sequence containing a GRE and its flanking nucleotide region in complex with the glucocorticoid receptor protein. They were able to characterize the atomic interactions between the protein and the DNA identifying binding structures and amino acids on the protein and specific nucleotides within the GRE and its flanking region. They are now beginning molecular dynamics simulations on the LTR nucleosome model with multiple glucocorticoid receptor proteins docked onto the five GRE sites (see part *d* of figure). This nucleosome 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. ■

Research Group

Pamela D. Popken-Harris, Research Associate

Michael R. Sullivan, Research Associate

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 nature 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 and 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 systems behavior.

This study examines the electromyographic (EMG) signal present in the urethral striated muscle during bladder function. ■

Dan Valleria, Principal Investigator

Antibody Modeling

This research group is synthesizing antibody fragments with the goal of making them usable in humans.

They are using Supercomputing Institute resources for computer modeling that will help the researchers optimize the fragments' binding ability. ■

Research Group

Xiaox Feng, Graduate Student Researcher

Ni Jin, Graduate Student Researcher

David Kuroki, Research Associate

Yangyn Shu, Research Associate

Deborah Todhunter, Research Associate

Mayo Medical School

Department of Pharmacology

Yuan-Ping Pang 243

Yuan-Ping Pang, Principal Investigator

Development of Second-Generation Farnesyltransferase Inhibitors as Cancer Drugs

The high prevalence of mutated Ras genes in human cancers makes Ras protein a suitable target for cancer drug development. One way to block the aberrant Ras functions is to inhibit farnesyltransferase (FTase), which modifies pro-Ras protein with the farnesyl isoprenoid lipid that is required for Ras protein's biological activities. Such inhibitors do not substantially interfere with normal cell growth, thus providing a promising approach to cancer chemotherapy. Indeed, first-generation farnesyltransferase inhibitors as potential cancer drugs are currently in Phase II clinical trials.

This research group's objective is to develop second-generation FTase inhibitors supplementing those currently in clinical trials with the aid of high-speed computing. Their specific aim is to identify FTase inhibitor leads by computationally screening chemical databases using an advanced docking program, EUDOC, that permits docking studies with metalloproteins and uses "spatial-decomposition" to achieve 100% parallelism. Five million druggable, commercially available compounds will be computationally screened against FTase by conducting a large-scale, high resolution docking study. The computationally identified leads will then be tested experimentally and optimized by using combinatorial chemistry and medicinal chemistry. ■

Research Group

Min He, Research Associate

Thomas Kollmeyer, Staff

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James D. Xidos, Staff

Metropolitan State University

Department of Information and Computer Sciences

Jigang Liu 245

Jigang Liu, Principal Investigator

Performance Evaluation of Parallel Computational Geometry Algorithms on the IBM SP

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 graphic user interface technology so that the user can freely define the scenarios for testing and evaluating purposes. The communication system is based on the UNIX IPC mechanism using TCP/IP protocol; it 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 computation geometry algorithms on the IBM SP supercomputer. ■

Minnesota State University—Mankato

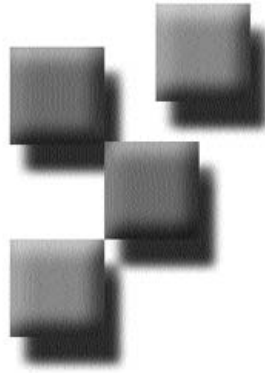
Department of Management

Rakesh Kawatra.....	247
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Rakesh Kawatra, Principal Investigator

Multiperiod Minimal Spanning Tree Problem— Formulation and Solution Methods

The Multiperiod Minimal Spanning Tree (MMST) 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 research suggests 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 solutions. ■



Index and Bibliography

Index of Principal Investigators

Bagrat Amirikian	224	Richard J. Goldstein	188
Ian M. Armitage	44	Anand Gopinath	165
Roger E. A. Arndt	151	Gautam Gowrisankaran	64
Leonard J. Banaszak	45	David J. W. Grant	76
George Barany	119	Alexander Grosberg	207
Avram Bar-Cohen	183	Rolf Gruetter	235
Victor H. Barocas	97	Satish Gupta	39
Bridgette Barry	47	Bojan Guzina	143
John C. Bischof	184	Franz Halberg	220
David A. Blank	120	J. Woods Halley	208
Victor Bloomfield	48	Shaul Hanany	210
Linda M. Boland	225	Lester Floyd Harris	238
Michele Boldrin	61	Joachim V. Heberlein	189
Charles E. Campbell	202	Stephen S. Hecht	217
Graham V. Candler	86	Dennis Hejhal	178
Robert W. Carr	99	John R. Hiller	37
Cynthia A. Cattell	204	Norton M. Hintz	211
Varadarajan V. Chari	62, 63	Kristin A. Hogquist	222
James R. Chelikowsky	100	James E. Holte	166
Bianca M. Conti-Fine	49	Miki Hondzo	145
Robert Cook	102	Thomas R. Hoyer	125
Germaine Cornélissen	220	Raymond M. Hozalski	146
Christopher J. Cramer	121	Wei-Shou Hu	106
Jane Davidson	185	Ioulia Ioffe	78
Gary A. Davis	139	Ashley James	88
H. Ted Davis	103	Rodney L. Johnson	230
Jeffrey J. Derby	104	Thomas W. Jones	95
Robert J. Dexter	140	Daniel D. Joseph	89
Mark Distefano	123	Steven Kass	126
Ding-Zhu Du	160	Rakesh Kawatra	247
Michael DuVernois	94	Yiannis Kaznessis	108
Linda B. M. Ellis	218	Michael P. Keane	63
David M. Ferguson	71	Paul Kiprof	35
Jürgen F. Fohlmeister	232	David B. Kittelson	191
Roger Fosdick	87	Katherine Klink	65
Efi Foufoula-Georgiou	153	Uwe R. Kortshagen	190
Catherine W. French	141	Daniel M. Kroll	72
Eric Ganz	206	Thomas H. Kuehn	191
Jiali Gao	124	Satish Kumar	109
Sean C. Garrick	186	Vipin Kumar	161
William W. Gerberich	105	Joseph F. Labuz	147, 148
Kristin Gillingham	237	Alex J. Lange	50
Steven L. Girshick	187	James Leger	167
William B. Gleason	219	Perry H. Leo	91

Kenneth Leopold	128	Lanny D. Schmidt	115
David Levitt	234	L. E. Scriven.....	117
Jack L. Lewis	228	William Seyfried, Jr.....	173
Perry Y. Li	192	Carol Shield.....	141,149
William Li	79	W. Thomas Shier	74
David J. Lilja	168	Nikolaos D. Sidiropoulos	171
John D. Lipscomb	51	J. Ilja Siepmann	130
Benjamin Y.H. Liu	193	Terrence W. Simon	198
Jigang Liu	245	Carl S. Smith	240
David Live	52	Charles C. S. Song.....	156
John S. Lowengrub	91,179	Masha Sosonkina	36
Thomas S. Lundgren	92	Friedrich Srienc	42
Mitchell B. Luskin	181	Heinz G. Stefan	157
Robert L. Lysak	212	Henryk K. Stolarski	148, 150
Christopher W. Macosko.....	110	Kumar K. Tamma.....	200
Krishnan Mahesh	93	Stanley A. Thayer.....	231
Susan C. Mantell	194	David D. Thomas	57
Kevin Mayo	53	Donald G. Truhlar	133
Richard B. McClurg.....	111	Dan Vallera.....	241
Alon McCormick	112	Oriol T. Valls	214
Peter H. McMurry	195	J. Thomas Vaughan	236
David C. Morse	114	Gianluigi Veglia	137
Karin M. Musier-Forsyth	129	Randall Victora.....	172
Ramaiah Muthyala	70	Carston R. Wagner	75
Douglas H. Ohlendorf	54	Kylie Walters	58
Hans G. Othmer	182	Dong Wang	40
Yuan-Ping Pang	243	Jon Weissman	164
James Pankow.....	81	Renata M. Wentzcovitch	118
Haesun Park	162	George L. Wilcox	226
Suhas V. Patankar	196	Carrie Wilmot	59
Maria German Paterlini.....	73	Darrin M. York	138
Christopher Pennell.....	223	David A. Yuen	174
Emil Pfender	189	Michael R. Zachariah	201
Fernando Porté-Agel	155		
Philip S. Portoghese	73		
David Y. H. Pui	197		
Shri Ramaswamy	68		
Diana Richards	66		
Osha Roopnarine	56		
P. Paul Ruden	170		
Yousef Saad	163		
Peter Santi	229		
Fadil Santosa	177		
Leonard S. Schultz.....	238		

Bibliography

January 1, 2001–March 15, 2002

(arranged alphabetically by field of study)

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