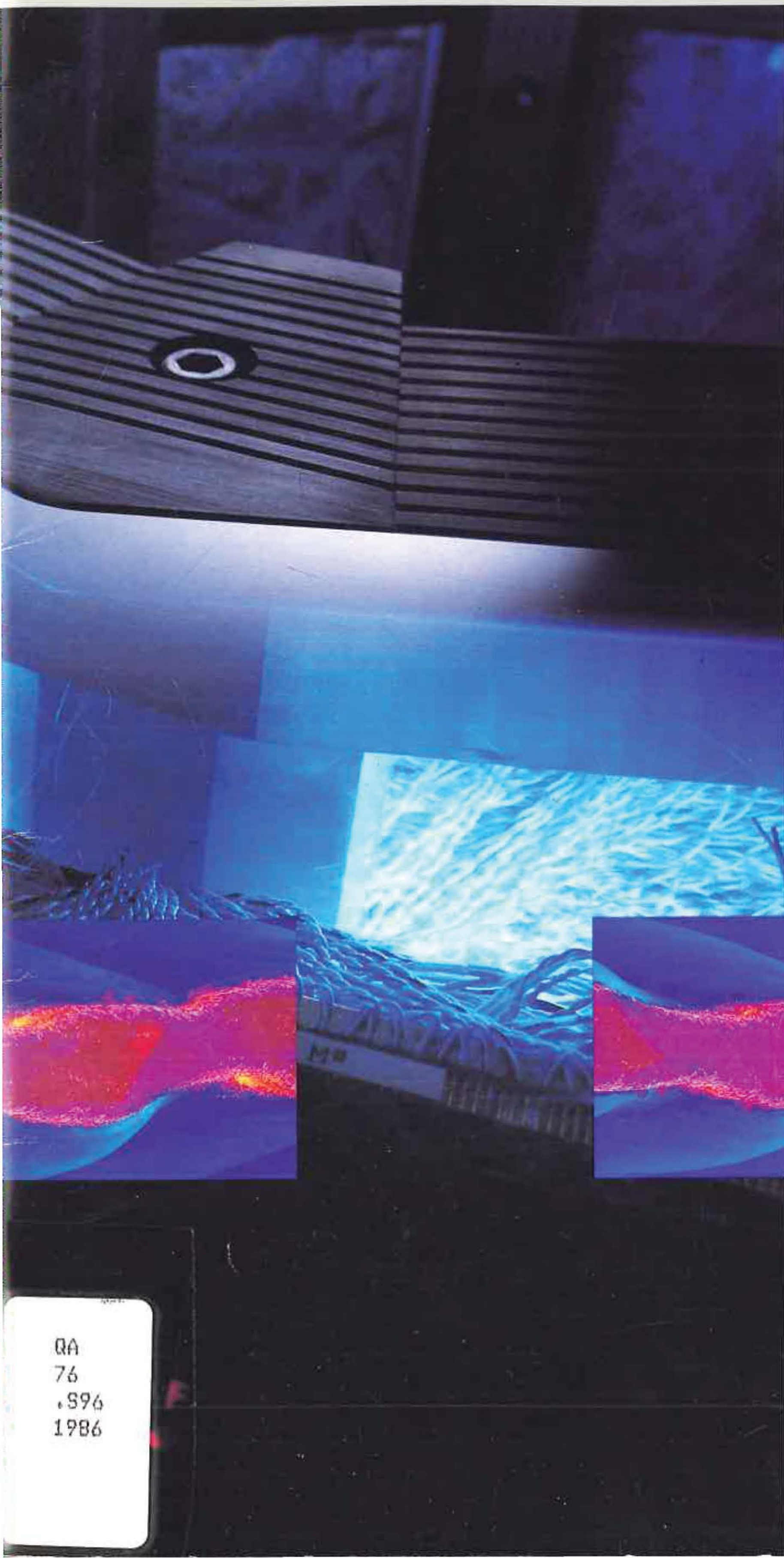
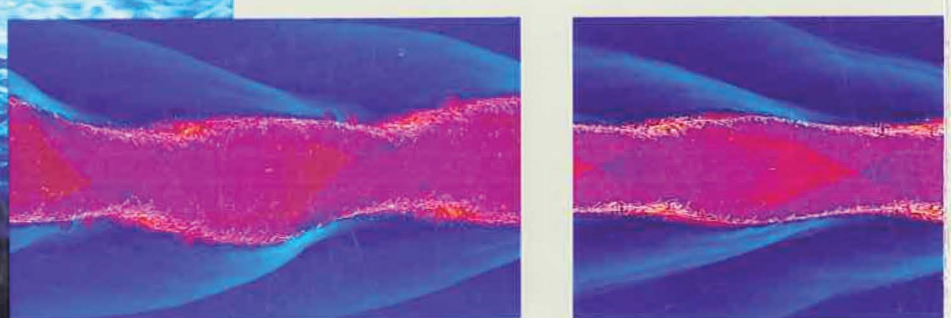
Supercomputing

at Minnesota

Carrying the Tradition into Tomorrow

University of Minnesota Computational Sciences Report





An elaborate cooling system is needed to dissipate heat produced by the 250,000 densely-packed microchips of the Cray 2 shown to the left. The large plexiglass columns in the background are reservoirs for the 3M Flourinert coolant, which actually comes in contact with the Cray's electronic circuitry—an approach thought impossible just a few years ago. Below, Minnesota Supercomputer Institute Fellow and University of Minnesota professor Paul Woodward and Thomas C. Jacobson, Director of Communications for Minnesota Supercomputer Center Inc., examine the display of a program running interactively on the Cray 2.

THE THIRD MODE OF SCIENCE

Why Is Supercomputing So Important?

Supercomputers attain their speed by processing information that has been vectorized, or assembled into arrays, instead of processing data in the sequential, step-by-step (or scalar) fashion of other machines. Their promise goes well beyond their ability to process data hundreds and sometimes thousands of times faster than conventional machines. Supercomputers, in fact, are changing the very nature of scientific research and experimentation.

The mathematical relationships that explain how the physical world behaves have been explored for decades. Now the speed of supercomputers can be used to study natural phenomena in ways that are otherwise impossible. Hypotheses can be tested and variables manipulated that would not be possible to test or manipulate in the laboratory. Supercomputing has led to the new field of computational science, sometimes called the "third mode" of science, that allows us to go beyond observation and theory and actually simulate natural phenomena. And since the enormous output of supercomputers can often be transformed into multi-dimensional graphic displays that change as variables change, scientists can in effect "see" processes that range from molecular interactions of exotic materials to the life cycles of stars. It has been said that with supercomputing we've entered an age in which information is not just processed, but *created* using numerical techniques that show us things never before seen by other means. This couldn't be more important. The effect has been compared to the impact the telescope had on the world view of 17th Century thinkers.

The supercomputer is no substitute for human creativity, imagination, or intelligence, but it amplifies those qualities in a manner that is having a major impact both on science and society.

Cover:

Close-up of a four-processor Cray 2. Inserts: Supercomputer simulation of the unstable oscillation of a gaseous jet. The jet is moving at a speed of Mach 4 through a gas of 10 times greater density.

CONTENTS

A Minnesota Tradition 2

A Chronology 4

The Minnesota Program Today 5

Research

— Physics 15

— Chemistry 16

— Chemical Engineering and Materials Science 17

— Astrophysics 18

— Mathematics 22

— Geophysics 23

— Mechanical Engineering 24

— Biomedical Research 25

— Electrical Engineering and Computer Science 28

— The Institute for Mathematics and Its Applications 29

— St. Anthony Falls Hydraulic Laboratory 29

— Economics and Management 30

— Agriculture 30

People 31

SUPERCOMPUTING

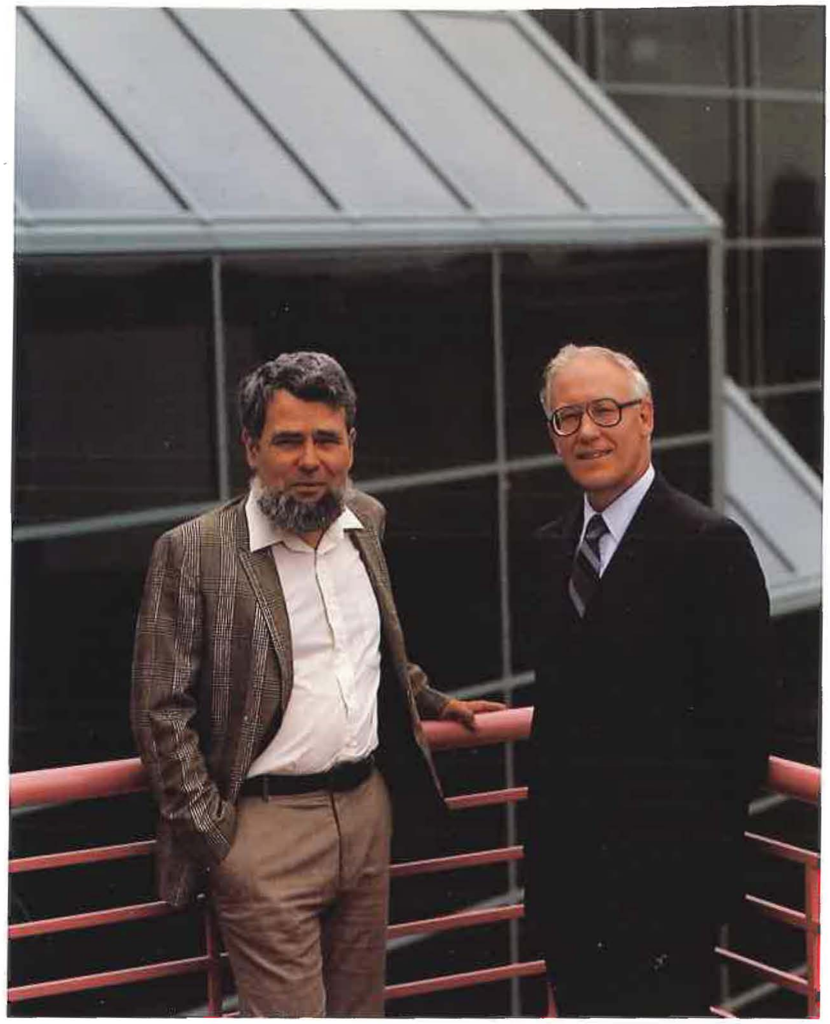
A Minnesota Tradition

The University of Minnesota has been a long-standing participant in the development of scientific computing, both by design and by virtue of our unusual circumstances. For one thing, we have been committed to making the most powerful computers available to researchers, both faculty and students — beginning with the Univacs of the 1950's.

Just as important is the fact that the developing revolution in supercomputing technology has been a uniquely Minnesota phenomenon, beginning with Control Data Corporation and Cray Research, and continuing with the addition of ETA Systems.

Because these companies are in our backyard, interchanges between supercomputer builders and the research community have been more frequent here than virtually anywhere else. Ideas have flowed back and forth easily. The latest generation of machines was and continues to be made available early to University faculty and students.

This University was the first academic institution to install a Cray 1 supercomputer, the first to operate two supercomputers, upon acquisition of the Cyber 205, and the first to install a Cray 2. The knowledge we have formed on this campus is extensive and growing daily. We've produced a place where supercomputer use is widespread, perhaps more so than at any other academic institution in the nation. Thousands of hours of access time have been used by hundreds of researchers and students. This has created a broad base of expertise at all levels, from students to senior researchers.



Minnesota Supercomputer Institute Director, Dr. Peter Patton (right), with Professor Thomas Walsh, Scientific Director. Patton is former director of the parallel processing program at the Microelectronics and Computer Technology Corporation; Walsh teaches at the University of Minnesota's School of Physics and Astronomy.

University researchers in physics, astrophysics, mathematics, geophysics, chemical engineering, materials science and chemistry all access the supercomputers through a high speed communications network. Programs in engineering, biomedicine, agriculture and business are growing rapidly and are connected to or will soon join this supercomputer network. The research communications network extends from the University campus to the new Minnesota Supercomputer Center, a facility that is unique in the nation, possibly the world.

The Minnesota Supercomputer Center is the cornerstone of the Minnesota Technology Corridor, a concentration of research and development facilities in a special development district located between the University campus and downtown Minneapolis. The Center houses:

— The Minnesota Supercomputer Institute, created by the University and funded by a special appropriation of the Minnesota State Legislature. The Institute's goal is to put Minnesota at the forefront of computational science and educate the students who will create tomorrow's technology.

— Minnesota Supercomputer Center Inc., formerly known as Research Equipment, Inc. This corporation was formed by the University in 1982 to support and manage supercomputer systems and provide for cooperative relationships with industry.

— University researchers and academic visitors from around the world, including many doing work sponsored by the National Science Foundation.

— Researchers and technicians from ETA Systems, Cray Research and other industrial partners.

— The most advanced collection of supercomputing hardware available to any academic institution.

The Minnesota Supercomputer Center results from the realization that large-scale computational science has become one of Minnesota's most valuable intellectual assets. It will help carry the Minnesota tradition of supercomputing into the next decade and beyond.

On a national level, supercomputers will help America maintain its competitive edge in areas where it is threatened, and quite possibly regain it where it has been lost. Some of that will happen at the Minnesota Supercomputer Center. The following pages provide an overview of the Minnesota program and some indication of where the work being done will lead in the years ahead.

Minnesota is home to all three of the nation's supercomputer builders. Control Data Corporation was a pioneer in large scientific computers. Today, its CYBER 205 is found in many of the world's leading research facilities. Cray Research was formed in the mid-70's by Seymour Cray, a former Control Data engineer. The Cray 2 vies with the CYBER 205 as the most powerful computer in the world. The newest entrant is St. Paul-based ETA Systems, which with Control Data's help is developing the state-of-the-art ETA-10. Above, ETA President Lloyd Thorndyke is shown holding one of the main processing units from the new ETA-10.

SUPERCOMPUTING AT MINNESOTA:
A BRIEF REVIEW

A Long Past in Tomorrow's Technology

1981: The University becomes first academic institution to install a Class VI supercomputer, the Cray 1.

1982: The University forms an affiliate, Research Equipment, Inc., to manage the supercomputers for academic researchers and provide cooperative opportunities for the industrial community.

1984: The Minnesota State Legislature appropriates $2.6 million in start-up funds for the Minnesota Supercomputer Institute. An additional $6 million appropriation per year is approved for the 1984-86 biennium.

1984: Supercomputing activity now involves more than 150 faculty and graduate students, representing over a dozen academic disciplines. The scope of this activity is unprecedented for an American university.

1984: The National Science Foundation designates the University, Purdue University and Boeing Computing Services as "Phase I" computing centers. These centers provide NSF researchers with access to Class VI machines. During 1984-1985, 149 NSF researchers, including University-based NSF grantees, use University supercomputers.

1984: The City of Minneapolis, the State of Minnesota and the University announce plans to jointly fund the Minnesota Supercomputer Center. The $11.5 million Center will be constructed in the newly-formed Minnesota Technology Corridor and will house the Supercomputer Institute, the Supercomputer Center management corporation, personnel from Minnesota's supercomputer manufacturers and students and researchers from around the world.

1985: The University acquires a Control Data Cyber 205 and becomes the first institution to operate two supercomputers. The agreement includes a later upgrade to an ETA Systems ETA-10. The large memory and highly vectorized architecture of the Cyber opens new doors to researchers.

1985: The first prototype Cray 2 is delivered, after discussions with Cray Research and Seymour Cray, an alumnus of the University, that began in 1982 and continued while the machine was under development.

1985: The second Cray 2 arrives, a four-processor machine that is faster and has more memory than any computer in existence. The high speed and giant memory of the computer provide further impetus to research.

1985: Work is completed on a campus communication network that links ten departments and schools with University supercomputers. The University begins using the industry-standard UNIX™ operating system for supercomputer work. UNIX™ makes it possible for PC's, workstations and terminals to "talk" with supercomputers in a uniform environment. Minnesota becomes the first academic institution with this capability.

1986: The 120,000 square foot Minnesota Supercomputer Center opens with the most advanced and extensive collection of supercomputer hardware available to any university. Research Equipment, Inc. changes its name to Minnesota Supercomputer Center Inc. to reflect its role as management corporation for the new facility.

1986: Several hundred researchers and graduate students are by now using University facilities to complete computational science research projects that range from the physical sciences to biomedicine, agriculture and economics. Dozens of papers have been published. Advances have been made in many different fields.

Overview and Operations

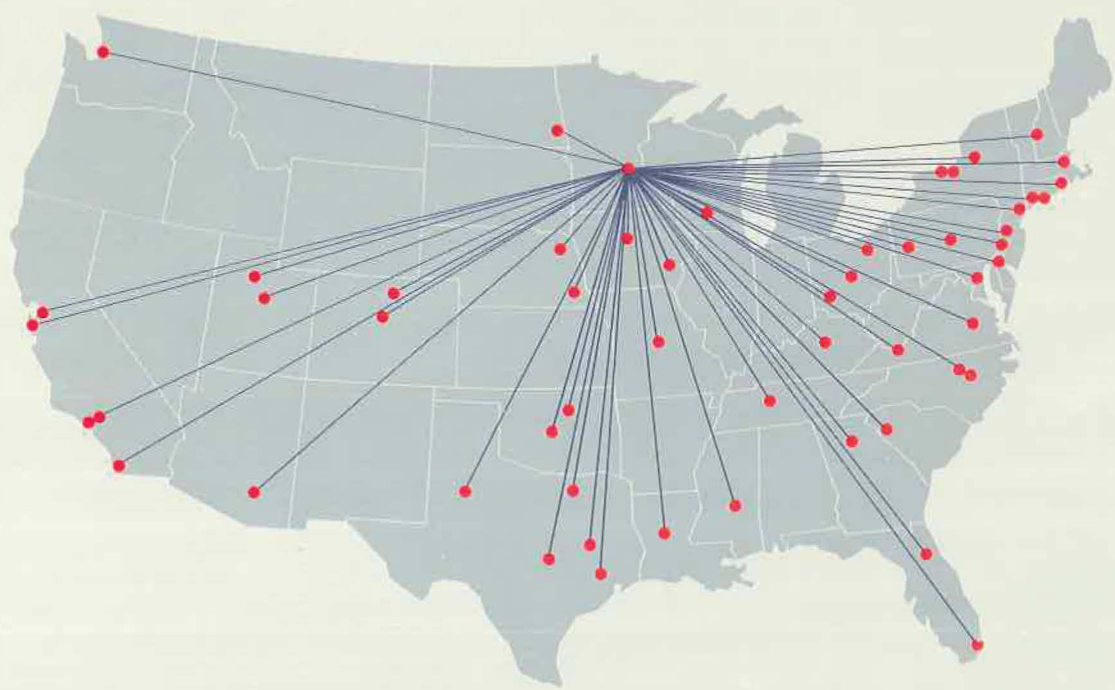
The Minnesota Supercomputer Institute

The Minnesota Supercomputer Institute was created in 1984 by the University of Minnesota with a special $6 million appropriation from the Minnesota State Legislature. It is an advanced scientific research organization designed to place Minnesota at the forefront of research and education using supercomputers. As a unit of the University of Minnesota, it is governed by the University's Institute of Technology, led by its Dean, Dr. Ettore Infante. Dr. Peter Patton, formerly director of the parallel processing program at the Microelectronics and Computer Technology Corporation, is the Director of the Institute and is responsible for scientific, educational, operational and administrative activities. As Scientific Director of the Institute, Professor Thomas Walsh of the University's School of Physics and Astronomy coordinates the research program he initiated in 1984.

The Institute is based on the concept of computational science as a research tool that cuts across all disciplinary borders. Fluid flow is an example. The same underlying physics and mathematics appear in astrophysical fluid flow, in aerodynamic fluid flow and even in the flow of blood in the human heart. As a unifying concept, computational science brings together these and many other fields at the point where they require the use of advanced computational techniques.

The multi-disciplinary focus can be seen in the backgrounds of five Minnesota Supercomputer Institute Fellows who were recruited to form the foundation of the Institute program and who hold joint positions with the University's Institute of Technology. The group includes: Professor Jan Almlöf (theoretical chemistry); Professors Aneesur Rahman and John Zabolitzky (condensed matter physics); Professor Paul Woodward (astrophysics); and Professor David Yuen (geophysics).

These five world-class computational scientists joined an active group of existing University faculty members who also hold joint positions as Institute Fellows. The expertise of the Institute Fellows ranges from the physical sciences to biomedicine and economics.



The National Science Foundation has embarked on an ambitious program to provide supercomputer access to the nation's leading researchers. Some of that access is provided by the Minnesota Supercomputer Center in a program being coordinated by the Center's management corporation. As this illustration shows, NSF researchers using Minnesota Supercomputer Center facilities represent most of the major academic and research institutions in the nation.

Architectural Graphics
— *Architecture*

Conduction Process During Contraction of the Mammalian Heart
— *Physics and Physiology*

Quantum and Classical Fluids
— *Physics*

Liquid Crystals and Spin Glasses
— *Physics*

Proton- and Pion-Nucleus Scattering
— *Physics*

Aperture Synthesis in Radio Astronomy
— *Astronomy*

Interaction Between Two Heavy Ions
— *Physics*

Low Temperature Reentrant Phase Transition in Granular Superconducting Systems
— *Physics*

Lattice Chain Melting
— *Physics*

Coulomb Glass
— *Physics*

Electrode-Electrolyte Interface
— *Physics*

Interplay Between Theory and Experiment in the "Hybrid" Area of Analytical Number Theory, Automorphic Forms and Selberg Trace Formalism
— *Mathematics*

Elastic/Plastic Fracture Mechanics
— *Aerospace Engineering and Mechanics*

3-D Ice-Sheet Model
— *Geology and Geophysics*

Large Scale Computations of Reacting Flows in Chemical Vapor Deposition Reactors
— *Chemical Engineering and Materials Science*

Rate Equations for Strangeness Production
— *Physics*

The Institute maintains a program granting supercomputer time on the Supercomputer Center systems to Minnesota faculty and visiting researchers. The grant program is extensive and spans a wide range of research fields. At one end is work involving the most timely and important research questions, often with national and global implications, that may require grants of between 50 to 500 hours time on a supercomputer. At the other extreme are smaller projects—a researcher wants to use a supercomputer in connection with an experiment or to analyze data collected elsewhere—that can be run quickly because of the speed of the hardware. Part of the Institute's charter from the State of Minnesota is to expand the use of supercomputers as widely as possible. Dealing with such a range of research demands may be complicated, but this type of flexibility is vital to the general usefulness of supercomputers in science.

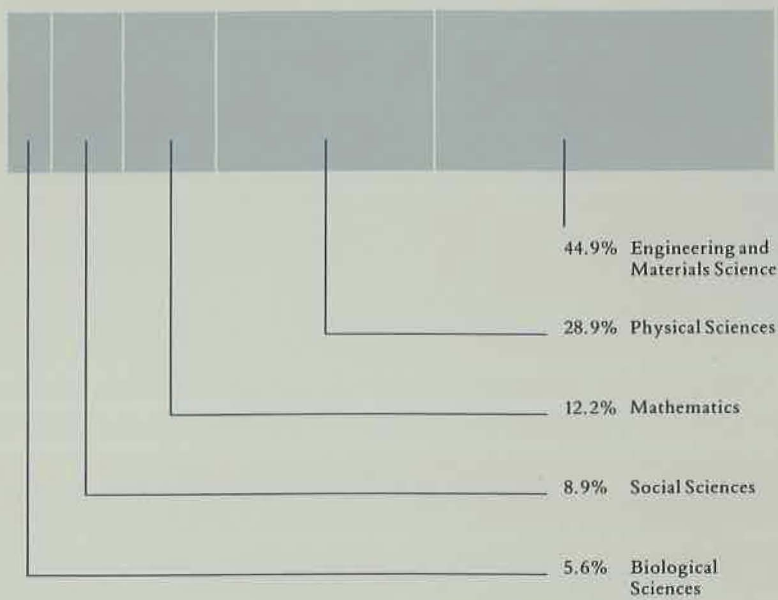
Since it has become widely recognized that scientific and technological progress in the next decade will be strongly influenced by access to state-of-the-art computers, educating those scientists and researchers who will make these advances has become a hallmark of the Minnesota advanced computing program. One reason for creating the Institute was to develop a large body of faculty and student researchers sophisticated in the operation and application of supercomputing for academic, industrial and government needs. This function stems from the tradition of graduate student involvement already strong on the University campus.

Currently, well over a hundred graduate students are doing thesis level work using the Center's facilities. The Institute supplies grants of supercomputer time for coursework in computational science and several Institute Fellows have developed extensive one-year computational science courses. In addition, through a large-scale purchase of workstations, a unique supercomputer learning center has been created on the University campus as a facility of the Institute of Technology.

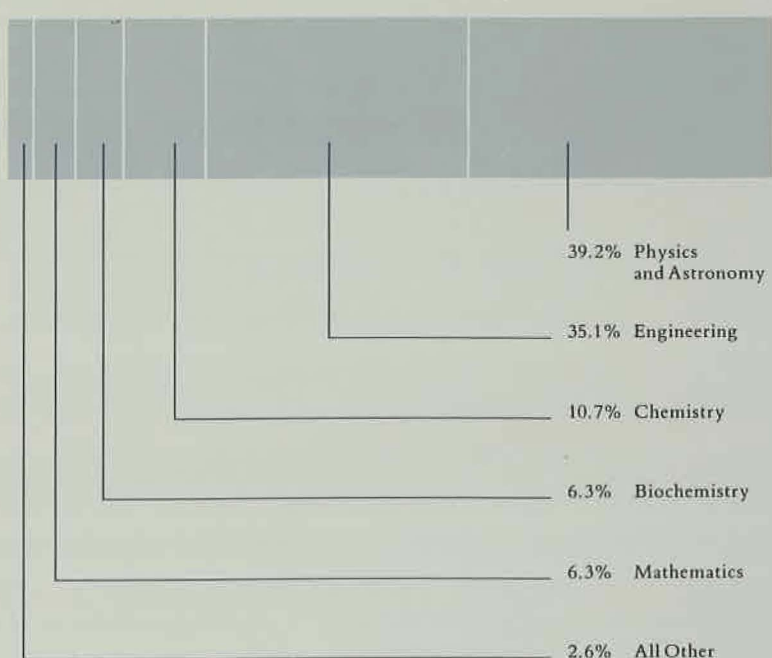
This breakdown of service units, which is a measure of supercomputer processor hours used, illustrates how National Science Foundation work being done at Minnesota spans a broad spectrum of basic and applied research areas, including the social sciences.

Due to both tradition and circumstances, supercomputer access has been more readily available to Minnesota faculty and students than perhaps at any other academic institution in the nation. Because the lengthy review process required by other institutions is often not appropriate at Minnesota, supercomputing has become an integrated part of campus research work. As the graph shows, the majority of that work is in physics, astonomy, and engineering.

Distribution of National Science Foundation Grants



Distribution of Minnesota Supercomputer Institute Grants



Representative Minnesota Research Projects

Fracture Mechanics, Composite Materials, Metal Forming, Tribology
— *Mechanical Engineering*

Nonlinear Partial Differential Equations and Theoretical Mechanics
— *Mathematics*

Space Plasma Physics
— *Physics*

Course: Numerical Simulation of Fluids and Plasmas
— *Physics*

MRI Brain Imagery in Three Dimensions
— *Medicine*

Development and Application of Numerical Techniques to Fluid Flow and Heat Transfer Problems
— *Mechanical Engineering*

Coating Flows and Processing Viscoelastic Liquids
— *Chemical Engineering and Materials Science*

Fluids and Process Technologies
— *Chemical Engineering and Materials Science*

Job Shop Simulation
— *Management Science*

Numerical Studies of Problems in Continuum Physics and Partial Differential Equations
— *Institute for Mathematics and Its Applications*

Velocity Field and Heat Transfer in Separating, Recirculating, and Reattached Fluid Flows
— *Mechanical Engineering*

Plunging Flow in Reservoirs
— *Civil and Mineral Engineering, St. Anthony Falls Lab.*

Nuclear Structure and Reactions
— *Physics*

Protein Simulation
— *Biochemistry*

Calculations for HF-HF Collisions and 3-Dimensional Reactive Scattering
— *Chemistry*

Improve Existing Simulation Codes Studying Natural Convection Heat Transfer Phenomena
— *Mechanical Engineering*

Quasiclassical Trajectory Studies of Inelastic Atom-Diatom Scattering
— *Chemistry*

Large-Scale ab initio Calculations of the Structure of Molecules
— *Chemistry*

Cosmic Ray Simulation
— *Physics*

Electronic Interactions at Metal/Semiconductor Interfaces
— *Chemical Engineering and Materials Science*

Cosmic Plasma Phenomena
— *Physics*

Laminar Flow of Thermosetting Polymer
— *Chemical Engineering and Materials Science*

Flow Field in Cyclone Separator
— *Mechanical Engineering*

Modeling of Airline Repair Facility
— *Management Sciences*

UM-SPICE Simulations of GaAs Circuits
— *Electrical Engineering*

Modeling Adjustments to School Transitions
— *Sociology*

Modeling of Group Processes
— *Sociology*

Modeling Packaging Lines in Process Industries
— *Management Sciences*

Viscous Flow with Flow Separation and Large Eddies
— *Civil and Mineral Engineering, St. Anthony Falls Lab.*

Transient Convection by Heat Loss in Lakes
— *Civil and Mineral Engineering, St. Anthony Falls Lab.*

Simulation of Biomolecular Dynamics and EPR Spectroscopy
— *Biochemistry*

Molecular Dynamics Simulation of Polymers in Small Pores
— *Chemical Engineering and Materials Science*

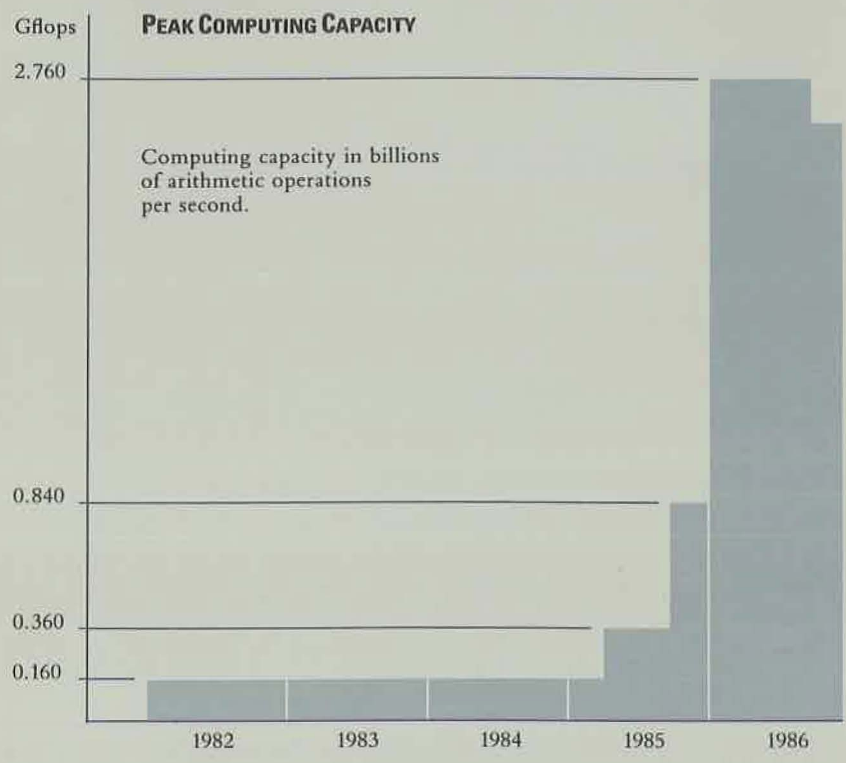
At the post-doctoral level, the University has worked closely with the National Science Foundation and other scientific organizations to make the facilities at Minnesota accessible to researchers from all areas of the country. The University was one of three "Phase One" centers designated by the National Science Foundation in 1984 to provide NSF-funded researchers access to the most powerful supercomputers. Since then, over 200 researchers have used University supercomputers as part of this on-going program. Minnesota expects to continue contributing to this national effort.

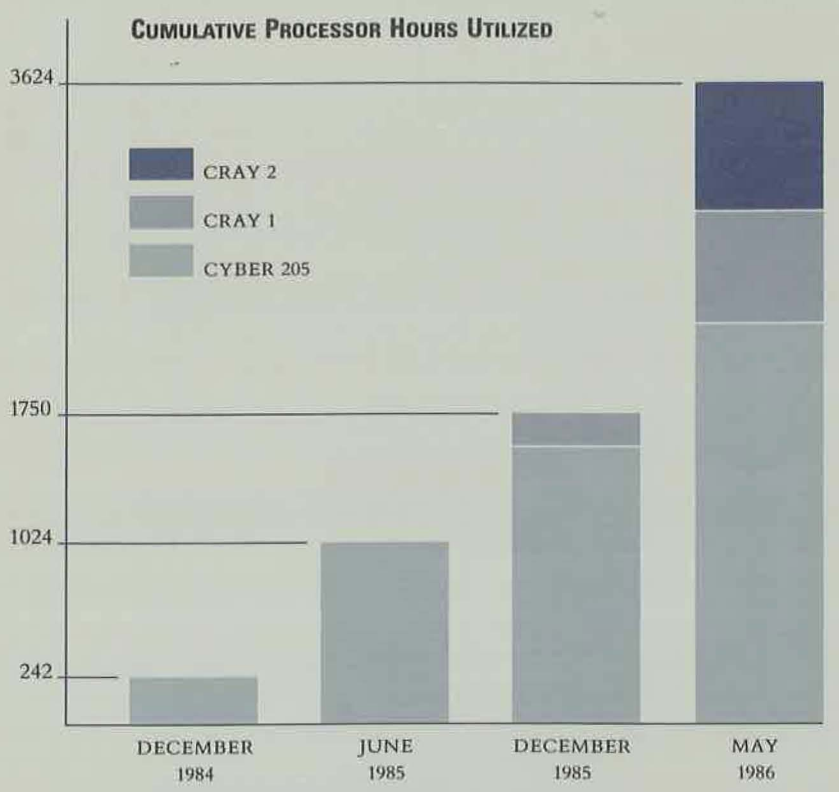
In addition, the Minnesota Supercomputer Institute hosts a unique Summer Supercomputer Program for graduate and post-doctoral students pursuing research sponsored by the National Science Foundation, as well as for industrial researchers. The second annual Summer Workshop will be held in cooperation with the Institute for Mathematics and Its Applications (IMA). This will be the first activity in the IMA's year long program dedicated to scientific computing. Participants in the intensive four-week session include both experienced and novice supercomputer users. Their backgrounds cover many areas of the physical sciences and engineering. Several aspects of the program are not found anywhere else, including the opportunity to gain familiarity with both Cray and Cyber systems and the chance to meet and learn from the researchers and technicians who are actually designing and building these machines. The program is an important first step toward establishing a national center for specialized instruction in supercomputing, both for graduate students in a broad spectrum of disciplines and for researchers, engineers and users of supercomputers in industry and government.

It is clear that the programs of the Minnesota Supercomputer Institute will help to foster University president Kenneth Keller's ambitious "Commitment to Focus" plan. Institute-sponsored research will continue to contribute to the University's reputation as an excellent advanced research center, as well as to the development of technology-based industry in the state.

Aggregate computing power available at Minnesota is the greatest of any U.S. university. A gigaflop is one billion calculations per second. The chart illustrates the dramatic rise in available gigaflops as new supercomputers were acquired.

The challenges that arise when new supercomputer systems are installed are both intellectual and technical. Each new generation of supercomputers bounds ahead of previous models in power and sophistication. The transition can be disruptive. The unbroken rise in cumulative processor hours used at Minnesota indicates that the resources are in place to handle such transitions smoothly.





Representative Minnesota Research Projects

Spinodal Decomposition in Binary Alloys and Fluids
— *Physics*

Plasma Physics of Earth's Magnetosphere
— *Physics*

How shapes of atomic nuclei affect the interaction between them
— *Physics*

Computation of vortex flow past a flat plate at high angle of attack
— *Mathematics*

3-D analysis of vibration isolation problems
— *Civil and Mineral Engineering*

Intermediate energy experimental nuclear physics: coupled-channel calculations
— *Physics*

Future of the turkey industry in Minnesota
— *Agriculture and Applied Economics*

Interaction between two heavy nuclei and the interaction between nucleons and nuclei
— *Physics*

Plasma simulation of an ion beam in an iconospheric plasma
— *Physics*

Development of a finite element program to analyze static and dynamic problems of reinforced composite laminates
— *Mechanical Engineering*

Time-dependent simulation of collisions of ions
— *Physics*

Mathematical modeling of stochastic hydrologic systems
— *Civil and Mineral Engineering*

Simulation of 3-D boundary value problems
— *Materials Science*

Natural building ventilation
— *Agricultural Engineering*

Cancer research
— *Medicine*

Representative Minnesota Research Projects

Elastic/plastic analysis of a centrally cracked thin rectangular plate under tensile loading
— *Aerospace Engineering*

Computations of reacting flows in thermal, plasma, and laser chemical vapor deposition processes
— *Chemical Engineering*

Interaction between a supersonic fluid jet and its surrounding medium
— *Astronomy*

Study of several heuristic algorithms for placement problem
— *Electrical Engineering*

Behavior of very long interconnections in silicon
— *Electrical Engineering*

Relativistic nuclear physics, six-part study
— *Physics*

Study of filtration characteristics of fibrous filters
— *Mechanical Engineering*

Course: Applied Numerical Analysis of Partial Differential Equations
— *Mathematics*

Continuous processing of reactive polymers
— *Chemical Engineering*

Development of numerical techniques for the solution of heat transfer, fluid flow, turbulence, and related processes in engineering applications
— *Mechanical Engineering*

Distributed VLSI design
— *Computer Science*

Fluid flow and heat transfer
— *Mechanical Engineering*

3-D molecular modeling study of the protein motions underlying muscle contraction
— *Medicine*

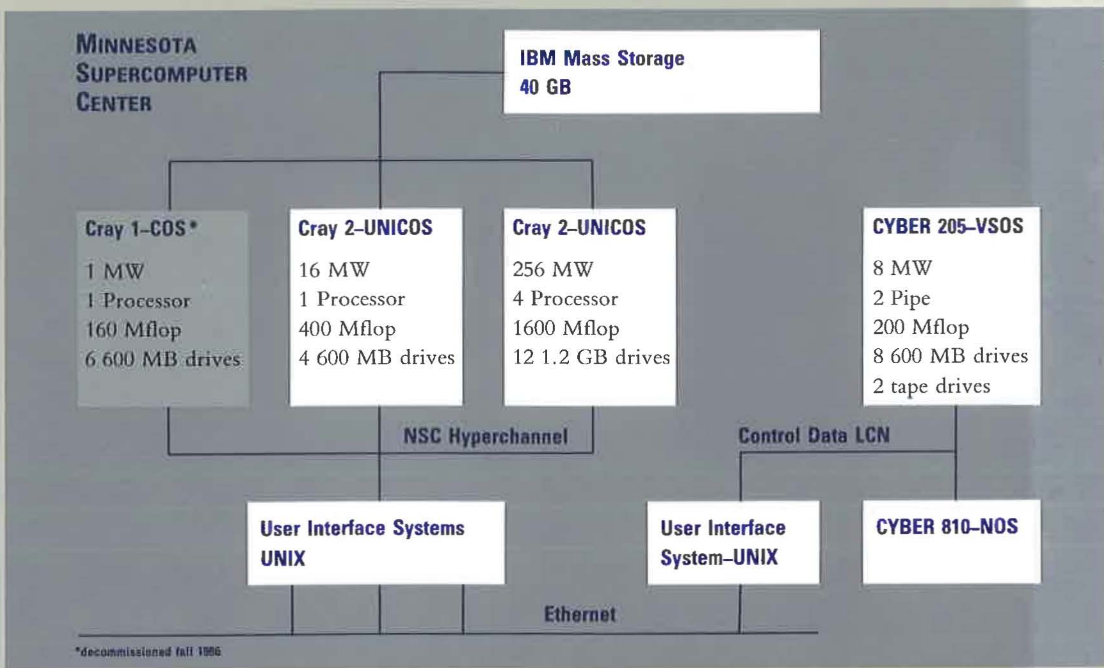
Econometric analysis of large systems of food expenditures
— *Agriculture and Applied Economics*

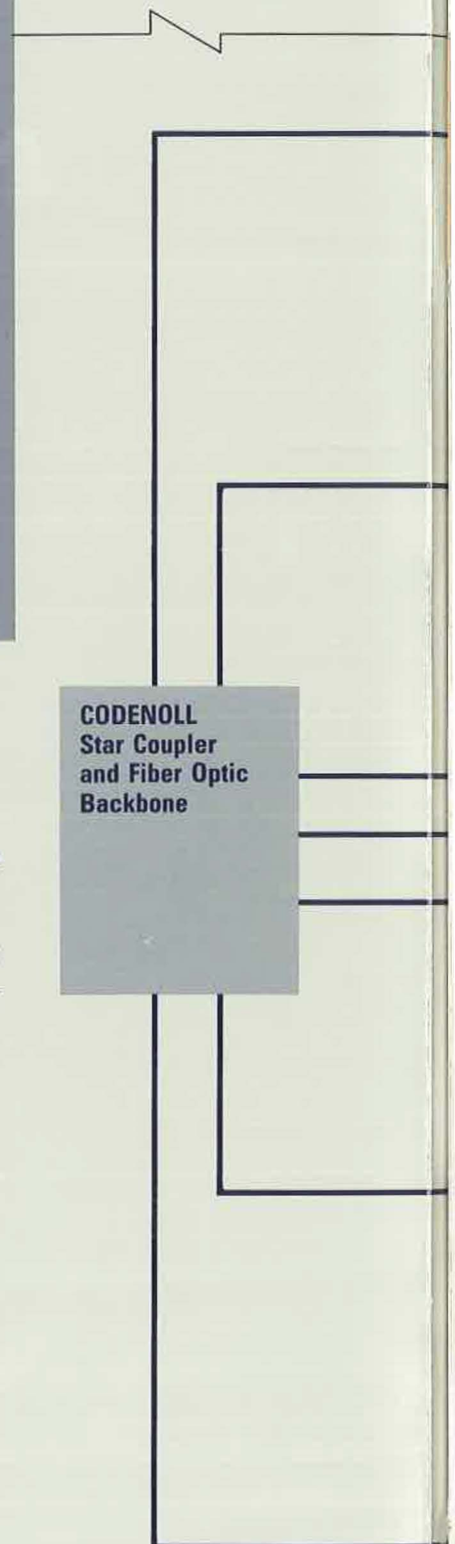
The Minnesota Supercomputer Center

The heart of the University of Minnesota's computational science program is the new Minnesota Supercomputer Center, an $11.5 million structure built adjacent to the University's campus in the emerging Minnesota Technology Corridor. The Corridor is a strip of land that connects the University with downtown Minneapolis. It is becoming a focal point for research and development activity in the Minneapolis/St. Paul area, one of the leading high-technology areas in the country. The Supercomputer Center is the Corridor's flagship project. It provides 120,000 square feet of office and computer space, with most of that space reserved for supercomputing activity. Some of the Center's more notable architectural features include a 60-foot crystalline atrium, indoor parking actually heated by the Center's computers, large conference and meeting areas and offices for visitors, and a 15,000 square foot, two-story high computer room with 66-foot clear span space and upper-level observation galleries.

Minnesota Supercomputer Center Inc., formerly known as Research Equipment, Inc., is the management corporation formed by the University to arrange the acquisitions of supercomputer hardware and to provide supercomputer services to the Minnesota Supercomputer Institute, the National Science Foundation, and the industrial community. This corporation operates the Minnesota Supercomputer Center and its supercomputer systems. It also works closely with Minnesota's supercomputer manufacturers, scientific researchers and industrial users to implement technical breakthroughs in software, network communications and various supercomputer applications that are making supercomputers more productive and easier to use today. In its unique position of serving both the research and industrial communities, this company has an excellent opportunity to further the transfer of technology from the University to the private sector.

Network access to supercomputers at the Center is widespread and as "transparent" as technology currently allows. Researchers in ten campus buildings connected to the Center are able to take advantage of the familiar UNIX™ operating system. This TCP/IP and Ethernet supercomputer access network is one of the most easily used and extensive in the nation. ▶





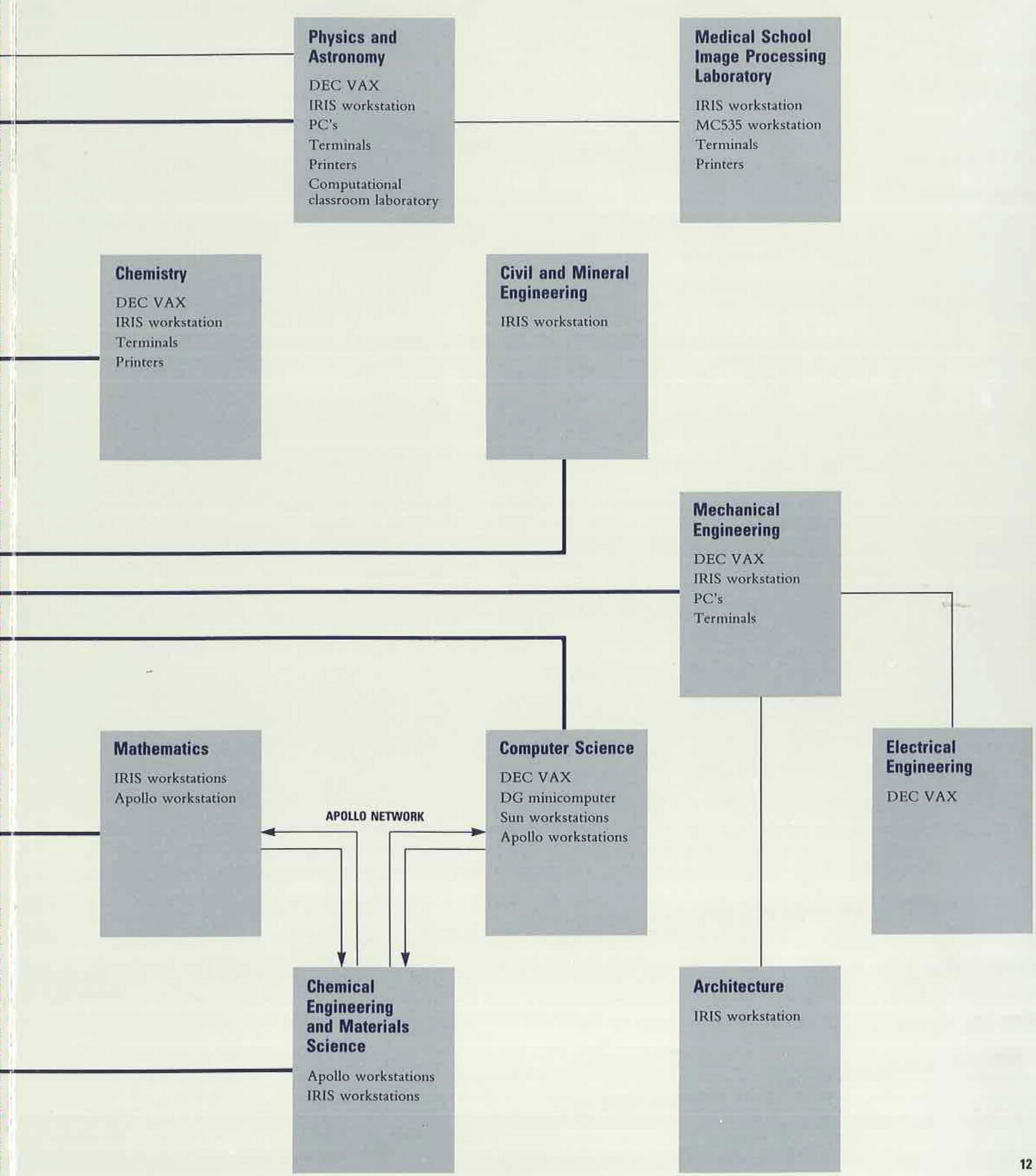
Minnesota's High Speed Campus Communications Network

Faculty and students at the University communicate with the supercomputers through a unique TCP/IP (Transmission Control Protocol/Internet Protocol) Ethernet system. This also gives researchers internet access to other scientists around the nation through the National Science Foundation's network. Minnesota has a growing expertise in TCP/IP network communications to UNIX™ supercomputers. In fact, the TCP/IP communications protocol runs directly on the Cray 2.

The system connects ten University buildings with the Center over a 10 megabit per second optical fiber network and local coaxial cable Ethernets. The optical fiber network uses a Codenoll Star Coupler to connect a system of fibers into a single transmission path. The network was developed by the Supercomputer Institute and the Supercomputer Center management corporation in cooperation with Bridge Communications. Connections to DEC and other equipment is through Excelan, Inc. products.

Silicon Graphics IRIS, Sun Microsystems, Apollo, Calcomp, DEC and IBM workstations and minicomputers are supported in a way that allows researchers direct and transparent access to the world's most advanced supercomputers. Researchers on campus have made animated films by transferring sophisticated graphics images from the Cray 2 to the Minnesota Supercomputer Institute IRIS workstations. These workstations are located at selected campus research nodes and form the Institute's principal color graphics display devices.

At the Center itself, in addition to Ethernet communications, different supercomputers are able to communicate at 50 megabits per second thanks to an ultra high speed backbone system developed by Network Systems of Minneapolis.


Physics and Astronomy
DEC VAX
IRIS workstation
PC's
Terminals
Printers
Computational classroom laboratory
Medical School Image Processing Laboratory
IRIS workstation
MC535 workstation
Terminals
Printers
Chemistry
DEC VAX
IRIS workstation
Terminals
Printers
Civil and Mineral Engineering
IRIS workstation
Mechanical Engineering
DEC VAX
IRIS workstation
PC's
Terminals
Mathematics
IRIS workstations
Apollo workstation
APOLLO NETWORK
Computer Science
DEC VAX
DG minicomputer
Sun workstations
Apollo workstations
Electrical Engineering
DEC VAX
Chemical Engineering and Materials Science
Apollo workstations
IRIS workstations
Architecture
IRIS workstation

The numerous workstations currently available may offer unique advantages to researchers in specific areas. Connecting these different systems in a supercomputer network is a hallmark of the Minnesota program. Silicon Graphics IRIS, Sun Microsystems, Apollo, Hewlett-Packard and Calcomp workstations have been successfully connected to the Cray 2 using the TPC/IP communications protocol.

Since its creation in 1982, the University's supercomputer management corporation has made notable contributions which have aided the growth of computational science at Minnesota. These contributions include:

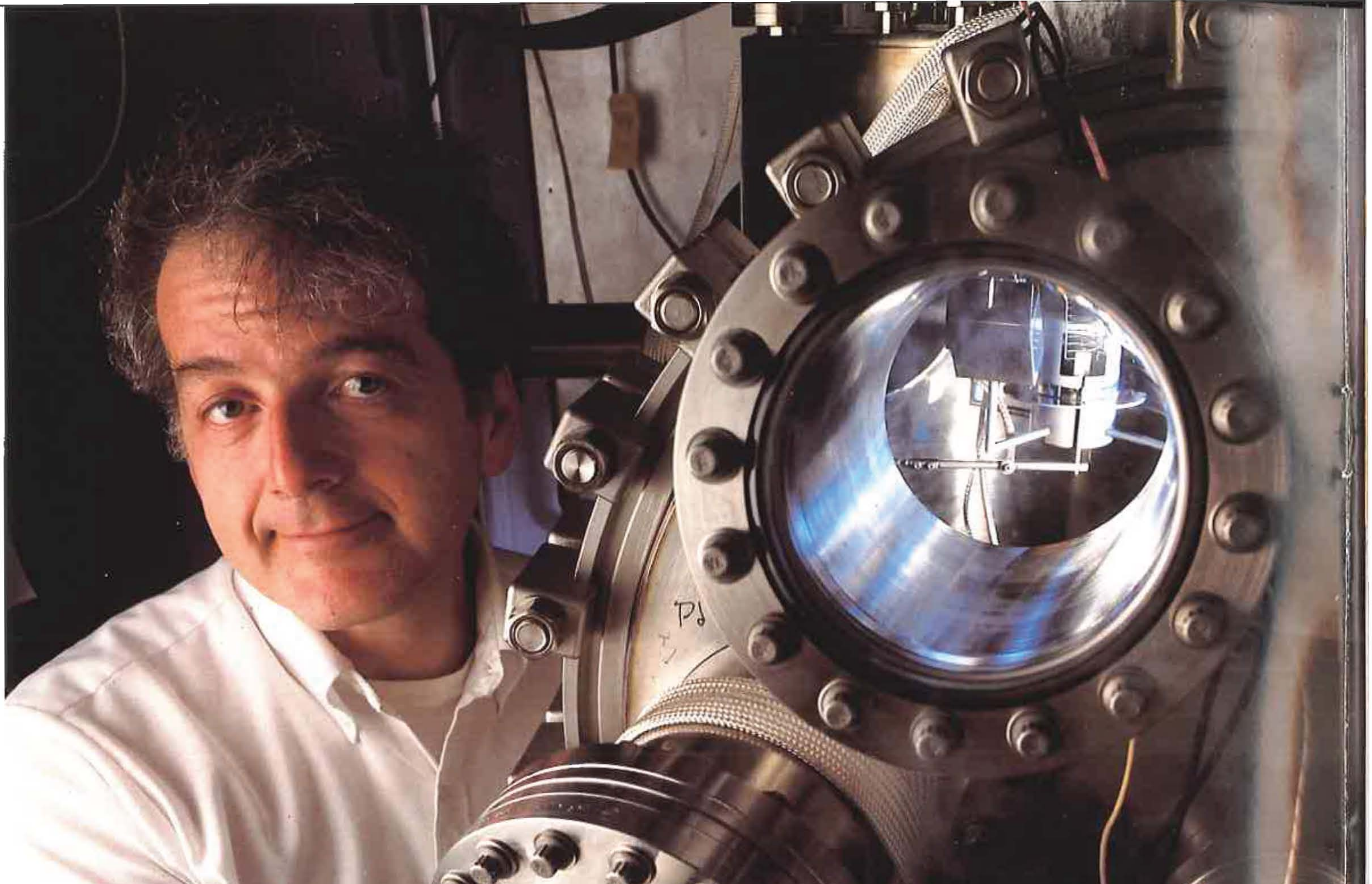
— Making a broad-scale commitment to UNIX™ access to the systems which it manages at the Minnesota Supercomputer Center. The first step was to employ UNIX™ as the operating system on the Cray 2.

— Developing and implementing a new UNIX™-based supercomputer mass storage concept (the XFS external file system), using inexpensive IBM 3380 disk technology.

— Developing the UNIX™ Remote Visual Editor, which allows efficient full screen editing on the Cray 2 using Silicon Graphics and Sun workstations within the campus network.

— Aiding the Minnesota Supercomputer Institute in the design and implementation of the campus-wide research network.

— Providing introductory supercomputer training for faculty and students as well as general user support and expert consulting.



University physics professor Allen Goldman exemplifies the remarkable closeness of supercomputer simulation and physical experimentation common at Minnesota. The device shown measures superconductivity at low pressure. Experimental results can be matched with observations from supercomputer simulations to produce a multidimensional approach to research that may revolutionize technology in the years ahead.

PHYSICS:

Using an Understanding of Many-Body Problems to Shape the Material World

In 1929, P.A.M. Dirac, one of the fathers of quantum mechanics, wrote, "The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known. The difficulty is only that the application of these laws leads to equations much too complicated to be soluble."

If Dirac had known of the computing power that would one day be available, he might not have been so pessimistic. With the help of supercomputers, computational physics is now at the threshold of overcoming this obstacle.

Since the structure and properties of atoms, molecules, gases, plasmas and fluids are due to electromagnetic interactions (basically, the repulsion of equal charges and the attraction of opposite charges), in principle the properties of *all* materials above the subatomic level could be computed from known physical laws. Unfortunately, any sample of a substance consists of countless atoms, all with many charges. Any detailed and quantitatively accurate descriptions of these systems involve the solution of immense *many-body* problems that must consider the interaction of thousands of particles.

Professors John G. Zabolitzky and Aneesur Rahman are discovering ways to solve these problems with the unprecedented computational power available at the Minnesota Supercomputer Center. By working out the equations that govern the basic microscopic interaction between particles, Zabolitzky and Rahman are making it possible to predict the properties of *macroscopic* materials, including materials that could significantly improve our lives.

Studying the behavior of many-body systems in computer simulations has many advantages over experimental studies. Measurements can be made without disturbing the object being measured. The "experimental" setting may be more tightly controlled within the computer than within the laboratory. Behavior not detectable in the laboratory can be gauged. Finally, researchers can modify parameters not easily modified in nature. By these means researchers can understand the origin of material properties from their underlying microscopic physics.

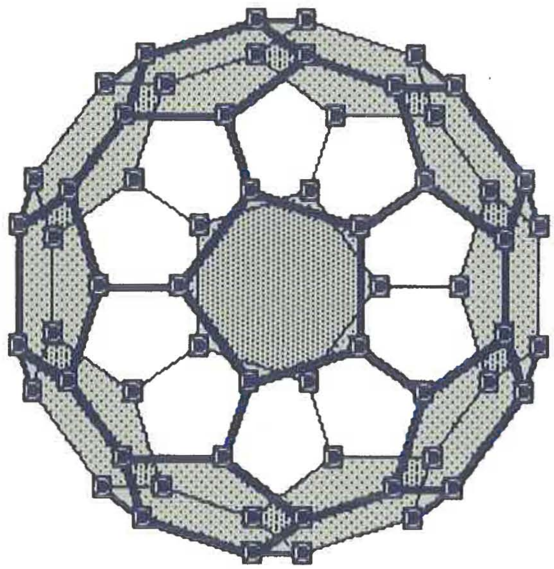
Work by Zabolitzky, Rahman and other researchers on the many-body problem has led to an understanding of many existing substances, from liquids to metals. The near future will see the application of this knowledge to produce new *computer-engineered* materials. A way to numerically represent the processes that make materials hard or soft, smooth or rough, more or less viscous, will lead to the production of materials that have the predefined properties society will need to meet the engineering needs of tomorrow.

Professor John Zabolitzky, School of Physics and Astronomy, is one of the five new Institute Fellows in computational science brought to the University to provide additional impetus to the research program. A leading researcher in theoretical many-body physics, he came to Minnesota from the University of Cologne.

Professor Aneesur Rahman, School of Physics and Astronomy, is one of the major figures in the field of condensed matter research known as molecular dynamics. Formerly with the Argonne National Laboratory, he is also one of five new faculty members and fellows of the Institute.

CHEMISTRY:

Solving the Vast Mathematical Puzzles of Quantum Chemical Behavior



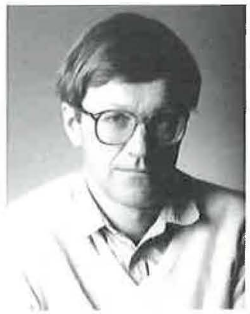
This amazing modification of a carbon molecule has caused a lot of controversy among experimental chemists. Is it stable? What will a more detailed structure look like and what will the molecule's other properties be? These questions are far from trivial, as such hypothetical forms of carbon could have important implications for the engineering of new molecular forms and substances. Quantum chemical calculations on the Cray 2 at Minnesota are likely to resolve the controversy.

Chemistry forms the basis for everything on which life depends. Understanding chemical processes has in the past been a matter of experimental laboratory work—work that has spanned centuries with results obvious to everyone. But the theoretical basis for all chemical behavior is quantum mechanics, the set of mathematical equations developed by Max Planck and others that attempts to explain physical processes at the atomic and nuclear levels. The mathematical complexity and intractability of quantum mechanics has meant that we have never been able to use these equations to analyze, understand and predict chemical behavior. If we could unlock the quantum mechanical secrets of chemical theory, molecules could be manipulated to form new substances that could potentially serve a wide variety of society's needs. Work being done by Professors Jan Almlöf and Donald G. Truhlar is doing just that.

Almlöf's and Truhlar's work involves modeling individual molecular reactions by using quantum mechanical principles. The work requires the 256 million 64-bit word memory available on the Minnesota Supercomputer Center's Cray 2 because the memory requirements of electronic structure calculations—a basic step in predicting intermolecular interactions—are enormous. Because memory banks of previous supercomputers were only 8 million words at most, the power of the Cray 2 is expected to bring a completely new dimension to theoretical chemistry.

The complexity of Almlöf's and Truhlar's work can be seen in the sheer numbers involved in modeling molecular dynamics. Mathematical equations describing molecular collisions are reduced to eigenanalysis and linear algebra and then "crunched" by the vector processors of supercomputers. One code developed at the University executes more than 112 million operations per second on the Cyber 205. The speed of this execution produced the first exact calculation of the probability of the transfer of a vibrational quantum (the smallest quantity of radiant energy) from one molecule to another. Thus, an important component of molecular interaction could be "seen" and predicted for the first time ever.

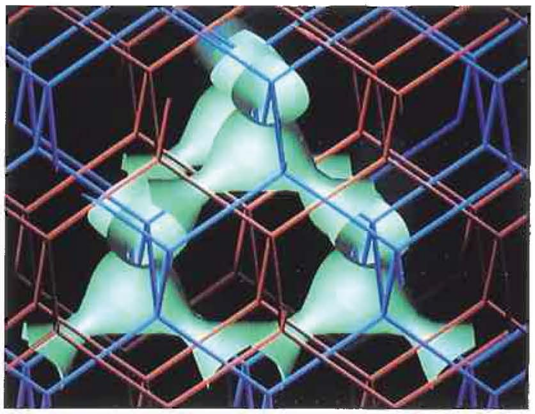
Since chemistry also underlies the life processes, computational quantum chemistry will play an essential role in the health sciences and biomolecular engineering. Now that we are developing ways to "see" what we once thought might be invisible forever, the potential for future developments is enormous.



Professor Jan Almlöf, Chemistry, is a leading expert on large scale chemical structure calculations. Formerly with the University of Oslo and now an Institute Fellow, he joins Professor Donald Truhlar, who is well known for his work on atomic and molecular scattering.

Chemical Engineering and Materials Science:

Mapping the Dynamic Patterns of the Materials of Modern Life



A supercomputer simulation of the surface between two liquids. The surface properties change depending on the concentrations of the liquids. The characteristics of this surface were explored by David Anderson as part of his doctoral thesis. Since the surface interfaces of such important substances as liquid crystals and polymer blends are only partially revealed by other methods, supercomputer simulation may reveal ways to manipulate these materials and create new and useful variants.

Many of the giant supermolecules (called macromolecules) that shape materials important to modern lives, including the polymers that form the basis for many man-made substances, are thought to be represented by hard, thin rods. Obviously, understanding how these rod-shaped supermolecules interact and under what conditions they change is of basic importance to the modern field of materials science.

To gain that understanding, researchers must consider the dynamics of systems of rods composed of as many as 1000 particles. Professors H. Ted Davis, Matthew V. Tirrell and graduate student Jules J. Magda are using Cray computers at the Minnesota Supercomputer Center to produce the most extensive simulations yet attempted of such systems, and as a result of their work, are forcing theorists into basic reconsiderations of the mechanisms of diffusion and rheology (the flow and deformation) in polymer solutions.

A research group headed by Professor Klavs F. Jensen is simulating another cornerstone of today's high technology—the production of thin solid films, such as single crystalline silicon and gallium arsenide, that form the basis for microelectronic processors.

These films are patterned into microstructure memories and signal switches when their substrates are exposed to gaseous chemical reactants in a process called chemical vapor deposition. The process involves complex interactions among fluid flow, heat and mass transfer, and homogeneous and heterogeneous reactions. Before, these interactions were evaluated through expensive and time-consuming laboratory experimentation. As the demand grows for microcircuits that perform more operations in less time, this experimental approach is proving increasingly expensive and difficult. Now through finite element analysis of models consisting of a large number of partial differential equations, Jensen and his group are using supercomputers to discover the patterns that govern chemical vapor depositions.

In a third representative area of materials science simulation, David M. Anderson, working under Professors Davis, L.E. Scriven and Johannnes C. Nitsche, used Minnesota Center supercomputers to simulate and display topographically-ordered surfaces on high-quality graphics terminals. This work contributed to an understanding of the microstructure of certain liquid crystals, microemulsions and polymer blends that are only partially revealed by x-ray, neutron scattering and electron microscopy. The work of Anderson and others shows that with the supercomputer, a potent new mathematical tool is emerging in America's efforts to maintain its lead in materials science and microelectronics.

Professor L.E. Scriven, Chemical Engineering and Materials Science, is an Institute Fellow and a leading researcher in the use of advanced mathematical and numerical methods to study problems in fluid mechanics, coating flows and process technologies.

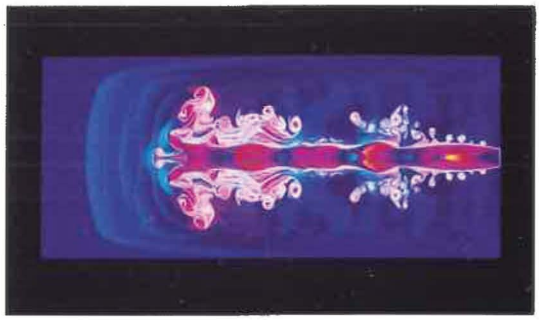
Left to right: Professor and department chairman H.T. Davis, and Professors M. Tirrell and K. Jensen.

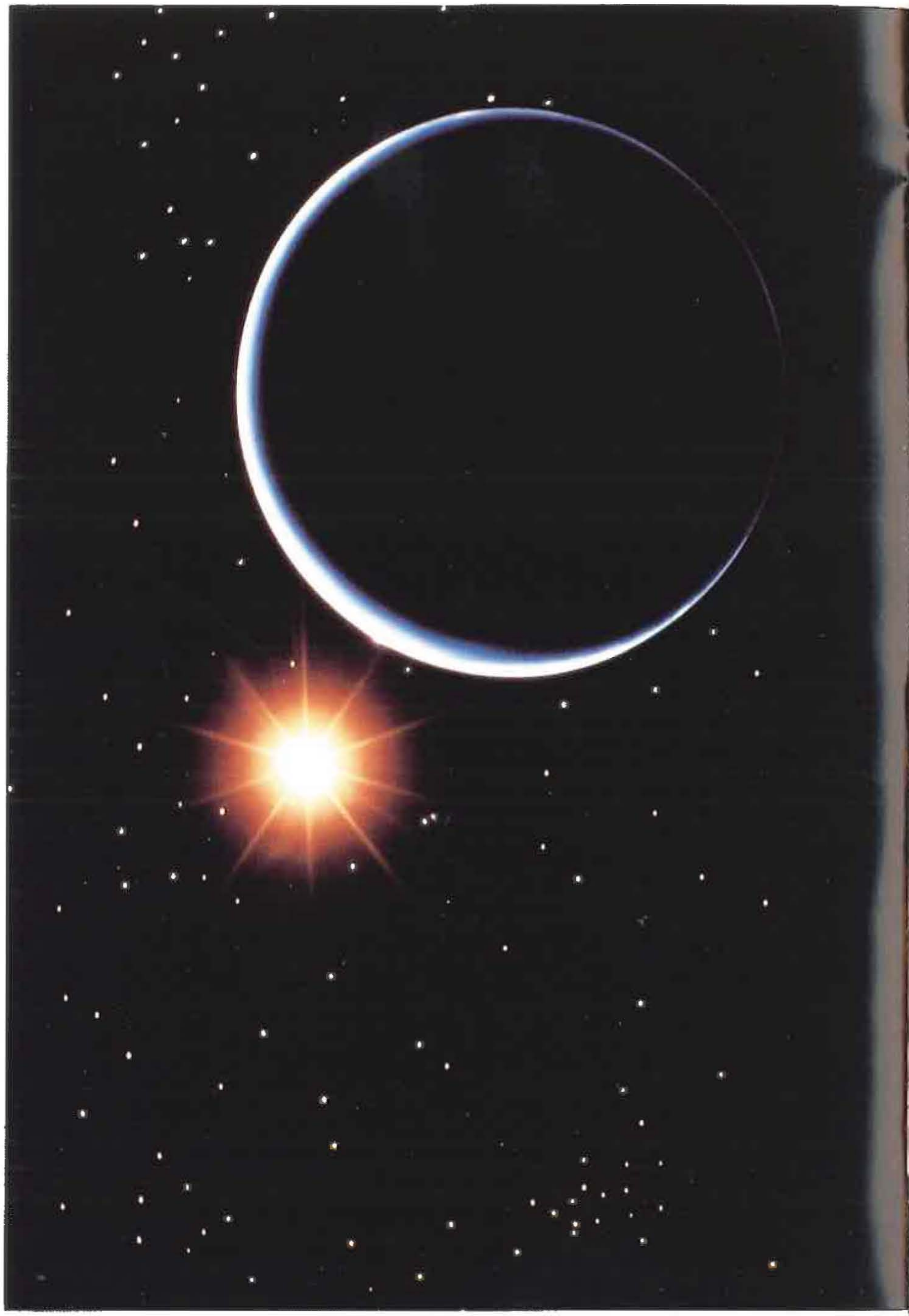
ASTROPHYSICS:

Numerical Tools to Probe the Evolution of the Cosmos

Great jets of matter have been observed streaming from the nuclei of distant galaxies. That events like these taking place hundreds of millions of light years away can be observed at all is one of the great achievements of 20th century science. But these observations are primarily morphological, meaning they provide information about the form but not about the physical nature of such galactic events and the ambient medium surrounding them.

Professor Paul Woodward, working with post-doctoral fellows David Porter and Marc Ondrechen, is using numerical techniques to simulate a variety of astrophysical systems, including the mysterious galactic jets. The best known of these techniques are the fluid interface tracking algorithm (SLIC), and the Piecewise-Parabolic Method (PPM), which were developed with collaborators at the Lawrence Livermore Laboratory.



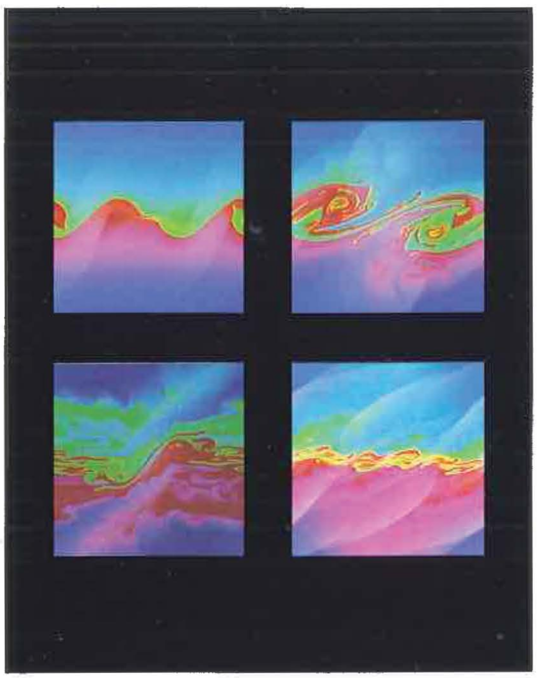


Simulation of the propagation of a gaseous jet through a medium of roughly the same density and half the pressure. As the density of the jet increases, colors change from yellow to red, purple, blue, and finally cyan.

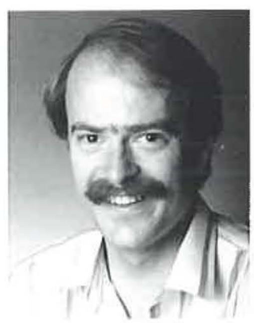
Using these techniques on the Cray 2, Woodward and his fellow researchers can simulate gaseous jets propelled to supersonic speeds and measure densities, temperatures and velocities at hundreds of thousands of locations. These simulations provide insights into the behavior of far more complicated flows—including the enormously powerful jets shooting out of active galaxies.

Further examples of the use of supercomputers in astrophysics are simulations that Woodward and Porter are making of compressible convection in stars. Convective transport of both heat and nuclear fuel play essential roles in the evolution of stars. Using Woodward's PPM code, simulations of this convection are leading to better models of stellar evolution and are helping to answer questions raised by more conventional forms of observation. Woodward's work has also inspired interest in using the PPM code to study other forms of turbulent flows, including thunderstorms in the Earth's atmosphere.

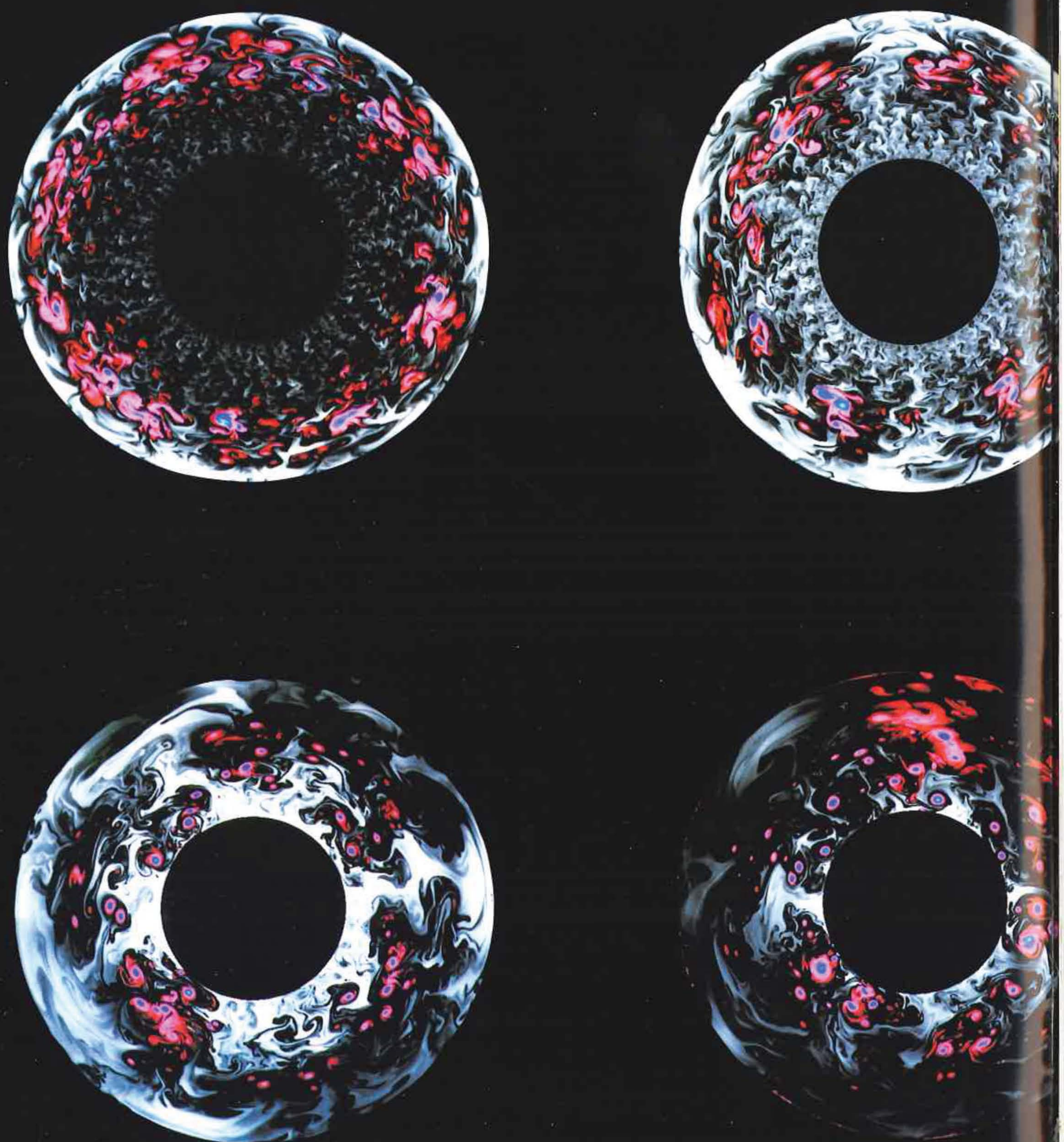
A final area of research employing the PPM code is the most spectacular. By using the PPM code to model the dynamics of interstellar gas, and a second powerful numerical technique, the Piecewise-Parabolic Boltzman code (PPB), to model the dynamics of stars, Woodward and fellow researchers are developing techniques to simulate 10 billion years of galactic evolution in a few hours time. The work may lead to an understanding of the evolution of spiral structures in disk galaxies. Woodward and his co-workers are showing that the computing power available at the Minnesota Supercomputer Center has the potential to significantly increase our understanding of the forces that shape the stars.



Set of four slip surface simulations. Shows the simulation of the unstable mixing of two gases at a boundary where they slip past each other at 2 and 4 times the speed of sound. Vortices and shock waves arise near kinks in this boundary.



Professor Paul Woodward, School of Physics and Astronomy, came to Minnesota from the Lawrence Livermore National Labortory, where he developed advanced numerical applications to fluid mechanics problems. He is one of five new faculty in computational science and an Institute Fellow.



Six snapshots of a developing convective flow computed on a Cray 2 by Woodward and Porter using the Piecewise-Parabolic Method. The computation simulates a very idealized model of convective heat transfer in stars. The annulus, or ring shape, is used to clarify the display. Colors represent gaseous temperatures. The relative temperature increases as the color changes from cyan to blue, purple, red, black, and finally to increasingly lighter shades of grey. The coloring of the data is due to the efforts of artist David Helder.

MATHEMATICS:

Supercomputers as an Aid to Insight

It's been said that of all the sciences, mathematics has been the least influenced by computers. According to this argument, mathematics may be the supreme intellectual exercise. As much philosophy as science, mathematics involves a painstaking mental search for general principles and does not substantially benefit from a computer's ability to "crunch" large amounts of data. Besides, the problems many mathematicians wrestle with involve proofs too vast for even computers to handle. Solutions often depend more on *insight* than on processing vast numbers of calculations.

Professor Dennis Hejhal, Mathematics, is an Institute Fellow who has led in the application of supercomputers as heuristic tools in the investigation of fundamental problems in pure mathematics. In the background are the historical original calculations of German mathematician Bernhard Riemann, who is best known for his contributions to the modern theory of gravity.

Changes in that attitude are shown today by Professor Dennis Hejhal, who is one of the few pure mathematicians in the country receiving National Science Foundation research support for use of a Cray supercomputer. Hejhal and Enrico Bombieri of the Institute for Advanced Study at Princeton, New Jersey, are using supercomputers at the Minnesota Supercomputer Center to break new ground in the area of pure mathematics called analytical number theory.

Specifically, Hejhal and Bombieri are putting Cray and CDC computers to work on one of the most famous unsolved problems in all of mathematics—the Riemann Hypothesis, which has deep implications for prime number theory and which has fascinated mathematicians for decades.

Hejhal and Bombieri are studying the behavior of zeros of Epstein zeta functions, a type of function closely related to the Riemann zeta function. "We are treating the Riemann zeta as a kind of black box whose insides are hidden," Hejhal told *Science 86*. "With the supercomputer we can give this box a good kick and then 'listen' as the zeros rattle around inside."

The goal is not merely the solution of an elegant but stupendous intellectual puzzle. Rather, by using supercomptuers, Hejhal is setting the stage for a whole new way of studying the finer properties of number-theoretical functions like the Riemann zeta. "For us," Hejhal says, "the primary goal of any supercomputer experiment is insight." This insight will ultimately, of course, be a product of the human mind, although supercomputing is showing just how far the mind can go.

GEOPHYSICS:

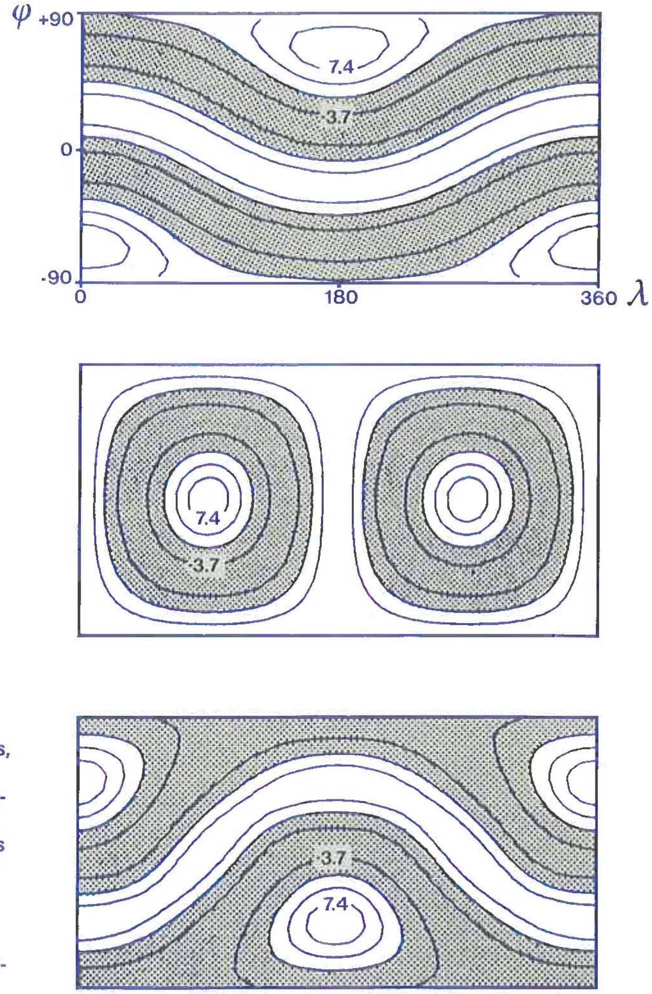
Understanding the Movements of the Earth Below Us

An earthquake may be over in a few seconds; the drift of the continents into their present positions has taken millions of years. Geophysicists attempt to understand the processes occurring within the Earth's interior that drive these and other events. By describing the dynamics of the earth's mantle, important questions can be answered about the large and sometimes spectacular forces that shape our world. New light can also be shed on such smaller but still critical issues as how the nature of geological structures will affect nuclear waste disposal sites or the motion of contaminated ground water.

Professor David Yuen and his graduate students are using the memory and processing speed of the Cray 2 at the Minnesota Supercomputer Center to develop convection models of the Earth's mantle. The goal is to understand the effects of radioactive heating within the mantle and the parameter values associated with mantle creep laws over periods of time ranging from seconds to eons.

The issues that Yuen's work addresses are linked to problems in other disciplines. Time dependence in thermal convection, for example, is important to fluid mechanics and nonlinear dynamics. Yuen is also using a three-dimensional model of the Earth's mantle to verify recent observations made on the spatial structure of the Earth's gravitational field, and to study the phenomena of double-diffusive convection, or the differences in convection rates of thermal and chemical layers within the mantle. Calculations at Minnesota have already determined the presence of thin chemical boundary layers embedded within thermal boundary layers.

These events may be happening hundreds of miles below us, but as Dr. Yuen and his graduate students are showing, simulation using advanced numerical techniques and the most powerful computers available may lead to a critical predictive understanding of the forces that are forming—and sometimes deforming—our world.



Professor David Yuen, Geology and Geophysics, uses modern numerical techniques to study convection, or the effects of heating, in the Earth's mantle. Formerly at the University of Colorado, Yuen is one of the University's five new faculty members in computational science and an Institute Fellow.

MECHANICAL ENGINEERING:

The Impact of Supercomputing on Tomorrow's World

The integration of large scale computing with applied mechanical engineering research promises a rich harvest of achievements in the years ahead. Using supercomputers in mechanical engineering will have an impact on such disparate design problems as optimal ventilation systems for office towers to diffusing heat build-up on the body of the proposed hypersonic space plane. Both involve problems of heat transfer, an area in which Professor Suhas Patankar has become a leading researcher. One of Patankar's concerns is heat transfer in electronic computer circuitry, which has become an increasingly critical engineering problem in today's small but circuit-packed supercomputers. Expertise being developed at Minnesota can play a role in the next generation of advanced computers now on the drawing boards.

Other researchers at Minnesota, often working in association with the University's industrial Productivity Center, are studying composite materials and simulating material fatigue and crack propagation in various structures. The latter problem is central to architectural engineering. How do cracks form in modern building materials and how do they propagate? Most importantly, how can such fatigue be stopped or minimized? Much of this simulation is being done in the Mechanical Engineering Department's advanced graphics laboratory, where graduate students and other researchers use three-dimensional models to study mechanical engineering issues and problems. A good example of the impact such work is having is a new software program now being developed by Professors Don Riley and S. Ramalingam, along with graduate student Jim Ellingson, which will allow engineers to simulate the injection molding or die casting of new manufacturing parts for the first time. In the past, through computer-aided design, engineers could create and perform a variety of analyses on a proposed part, but had to wait six to 18 months to see if the part could actually be manufactured. Thanks to work being done at Minnesota, the manufacturing process itself can now be simulated, greatly reducing the lag time between the design of a part and its successful production.

The Mechanical Engineering computer graphics laboratory developed by Professor Don Riley. This department, one of the leading research groups in the nation, is rapidly moving into computer simulation of mechanical engineering problems.

Professor Suhas Patankar (left), an Institute Fellow, has for several years developed supercomputer solutions to heat transfer and fluid mechanics problems. Professor Don Riley (right), is working with the department's Productivity Center to improve supercomputer simulation of manufacturing processes.

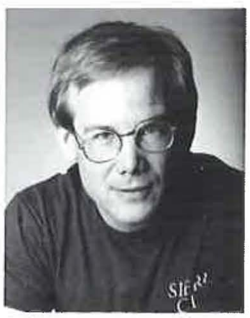
Finding the Biomolecular Patterns that Underlie Life

The last few decades have seen an exponential increase in research on the secrets of the human body. The goal is knowledge that not only describes, but explains and *predicts*. Researchers have begun to incorporate physics, mathematics, chemistry and other fields into their experimental approaches. Much of this transition from biology to *bioscience* has depended on sophisticated mathematical procedures to reveal the relationships between the data produced by the rapid pace of research. But the patterns that determine the form and substance of biomolecules, and ultimately, of the bodies they form, can sometimes be determined only when millions of variables are compared.

The efforts of Professors David Thomas and George Wilcox reveal how supercomputers can shed new light on the workings of the body. Dr. Thomas has generated a simulation sequence on the Cray 1 that models the mechanics of the molecules responsible for muscle contraction. Muscle movement occurs because complexes of large protein molecules form filaments that convert chemical energy into motion. This supercomputer simulation shows the predicted behavior of the energy-utilizing heads of these macromolecular filaments. This type of simulation permits Thomas to predict how molecules interact to allow organs to function.

Biomedical research using Minnesota Supercomputer Center machines will also examine the chemical mechanisms of the normal and abnormal regulation of cell function. Presently, researchers around the world can decipher genetic codes and predict the amino acids those codes determine. Ultimately, knowledge of the majority of genes and their products will permit a mechanistic—and predictive—explanation of many aspects of cell function and dysfunction. But the data base of known genetic sequences today is vast, and the prediction of structure from sequence is not presently possible. An understanding of the control of cell growth and such diseases as cancer will require breakthroughs in this area of biology.

Professor George Wilcox, Pharmacology, is leading a new initiative at the University of Minnesota Medical School to develop supercomputer applications in biomedical research. He is associated with the Biomedical Imaging Processing Laboratory, supported by the National Institute of Health.



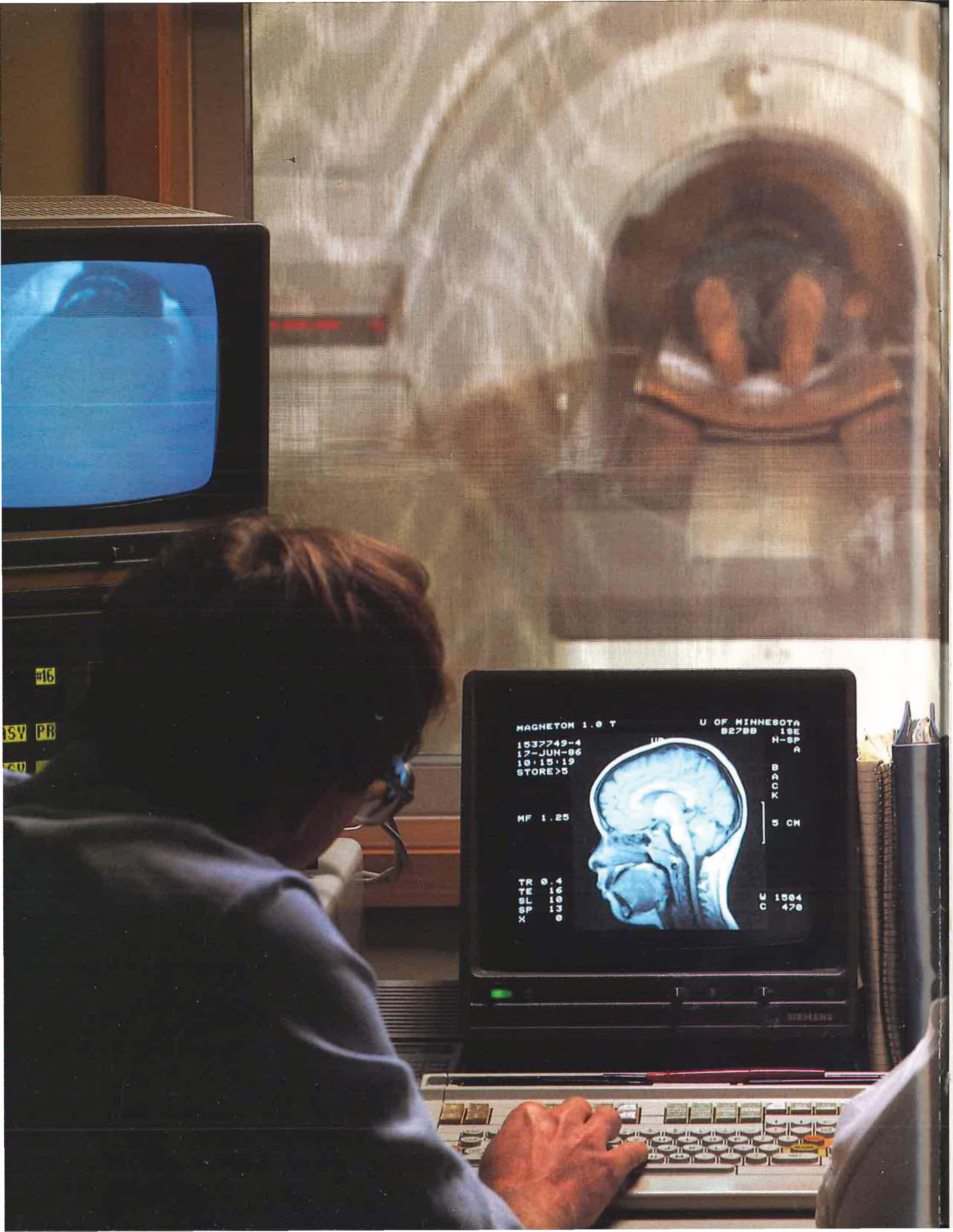
Professor David Thomas, an Institute Fellow, has carried out extensive supercomputer modeling of protein structures in solution on the University's Cray 1, Cray 2 and CYBER 205. Like other researchers at the University, he combines simulation with laboratory experimentation.

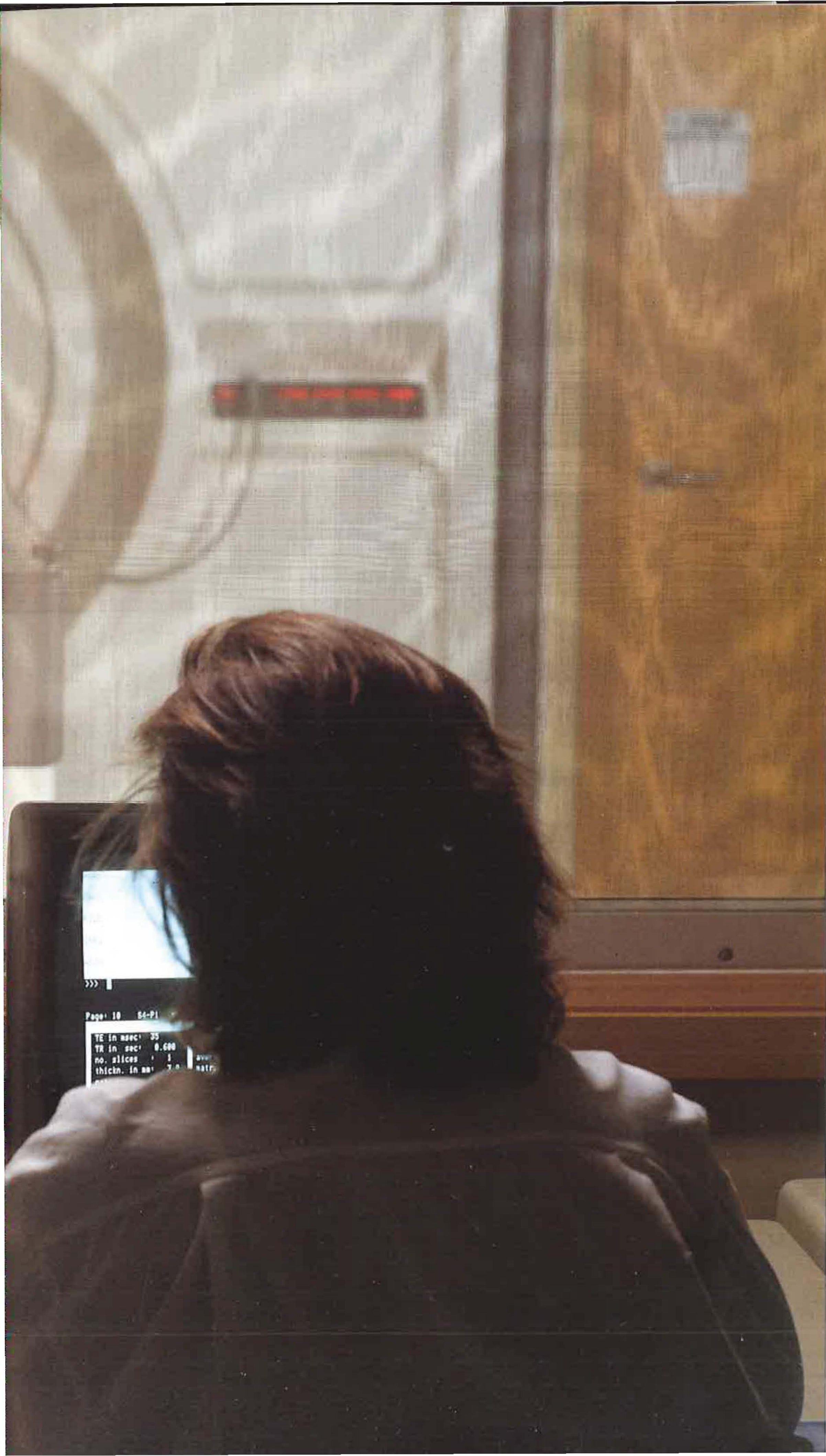
University researchers in collaboration with Dr. Wilcox will use supercomputers to compare newly discovered sequences, letter by letter, with the growing library of thousands of sequences. They will then use sophisticated graphics workstations, linked to the supercomputers, to estimate the structure of newly-sequenced proteins by comparing them to previously-defined proteins. This technique may make prediction of protein structure possible in the near future, but it will require mathematical models of unprecedented complexity and the processing power of the most powerful supercomputers.

Supercomputers are also being used to enhance the power of today's most powerful diagnostic tools. Sequences of two-dimensional images from CAT scanners, video microscopes and other digital imaging machines can be reconstructed into more revealing three-dimensional images when a supercomputer is used to reprocess the millions of picture elements involved.

The application of digital processing to problems in biomedical research will open doors of understanding not imagined even a few years ago. To begin opening these doors, Minnesota scientists are collaborating with the Minnesota Supercomputer Center in many areas of digital biology. The work ranges from the molecular modeling of new drugs to the scanning and mapping of tissue by the mathematical manipulation of tomographic data. As greater processing speeds and memory are made available by the Supercomputer Center, researchers will come to understand even more of the mechanics of life.

One view of a 3D reconstruction from 48 CT scans of a woman's pelvis. Image prepared using a Pixar Image Computer and reprinted with permission from Pixar. Pixar Image Computer is a trademark of Pixar. Copyright © 1984-1986 Pixar. All rights reserved.


#16
MAGNETOM 1.0 T
U OF MINNESOTA
1537749-4
17-JUN-86
10:15:19
STORE>5
BACK
MF 1.25
5 CM
TR 0.4
TE 16
SL 10
SP 13
X 0
W 1504
C 470



Magnetic Resonance Imaging (MRI) of the human body is a rapidly developing diagnostic tool. When University supercomputers are used to reconstruct three-dimensional images from data from MRI devices, previously hidden structures can be revealed.

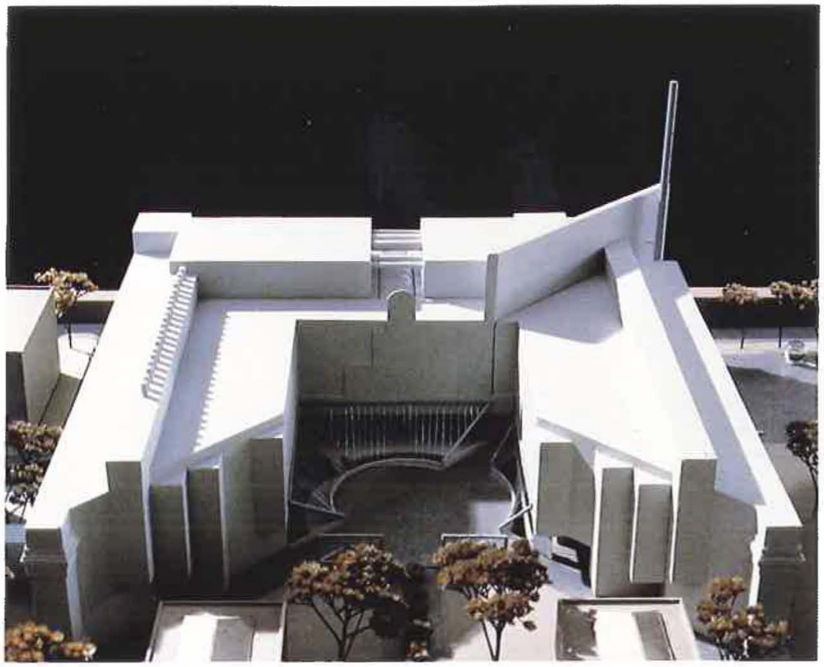
Electrical Engineering and Computer Science

In addition to the work we've just seen, many other supercomputer-based research programs at Minnesota are growing in prominence and potential. Several are poised to have a major impact on emerging technologies in the world beyond the laboratory.

In electrical engineering, for example, Professors Michael Shur, Bruce Bernhardt and Jingming Xu have transformed the popular circuit-simulation program SPICE into UM-SPICE, which for the first time allows circuit designers to simulate gallium arsenide circuits on workstations that communicate with supercomputers. Many believe GaAs will replace silicon as the basic substrate of digital circuitry because it offers substantial performance benefits. But before that happens, researchers will have to gain a better understanding of the novel properties of GaAs, and circuit designers will need to "retool" software to take advantage of this new material's potential.

Shur and fellow researchers are studying the way electrons travel through GaAs crystals. Their work is being done in cooperation with the Microelectronics and Information Sciences Center (MEIS), an organization jointly established by the University and leading Minnesota high technology companies to coordinate and fund research programs. Industrial participants include Honeywell, 3M, Cray Research, Sperry, Control Data, ADC Telecommunications, Zycad and VTC, Inc.

With UM-SPICE, Shur's group has successfully adapted a program that was designed to simulate small silicon-based circuits on PC's and workstations to one that can simulate much larger and more complex GaAs circuits—calling on a supercomputer via a communications link when the supercomputer's power is needed. This configuration may be a prototype of the design station of the very-near future, when the desk-top PC serves as a vehicle for initial exploration, and as a supercomputer workstation when large scale computer power is needed.



A model of the new Institute of Technology building for the departments of Electrical Engineering and Computer Science. This new facility is now under construction and is part of a major University commitment to these important fields.

Under the direction of its chairman, Professor David Fox, the Department of Computer Science is exploring many other areas involving both supercomputers and multi-processor parallel computers. Currently, the National Science Foundation is funding work to develop new techniques and algorithms that will make both computing environments more efficient and productive. Along with the Minnesota Supercomputer Institute, the Department of Computer Science is actively involved in training graduate students in the critical area of computer networking and was instrumental in developing Minnesota's supercomputer campus network.

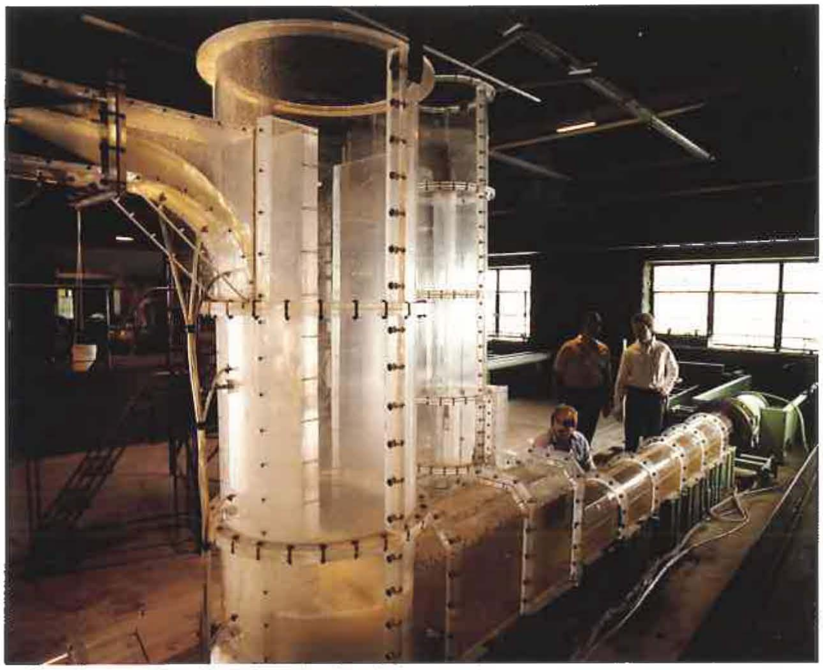
The Institute for Mathematics and Its Applications

In the past five years, the National Science Foundation has established the Institute of Theoretical Physics (ITP) at the University of California at Santa Barbara, the Mathematical Sciences Research Institute (MSRI) at Berkeley, and the Institute for Mathematics and Its Applications (IMA) at Minnesota. The goal was to stimulate interaction between junior and senior researchers in various disciplines and create healthy environments for postdoctoral training.

The IMA was recently funded for a second five years, in part because of the opportunities the Minnesota Supercomputer Institute has been able to provide in applying supercomputer power to mathematical research. A good illustration is work being done by Professor Mitchell Luskin of the School of Mathematics and a team of graduate students. Luskin and fellow researchers are using the Cray 2 to simulate the properties of liquid crystal configurations, which today are most commonly used in wrist watches, but which have the potential to replace many kinds of bulky optical displays—including color video displays. The mathematical properties of liquid crystals are also fascinating to mathematicians.

Previous research has explored the energy levels needed to activate simple liquid crystal displays, but a lack of appropriate algorithms and insufficient computing power meant that only small configurations could be be studied. Luskin and fellow researchers are using the Cray to simulate large and complex configurations and are paving the way for the development of new applications of the optical properties of liquid crystals.

Luskin is also working with IMA associate director Professor George Sell on work that may have a similar impact on applied technology—developing numerical solutions to the mathematical equations that govern the movement of recording heads over magnetic media, which may lead to discoveries of more efficient ways to magnetically record and retrieve data.

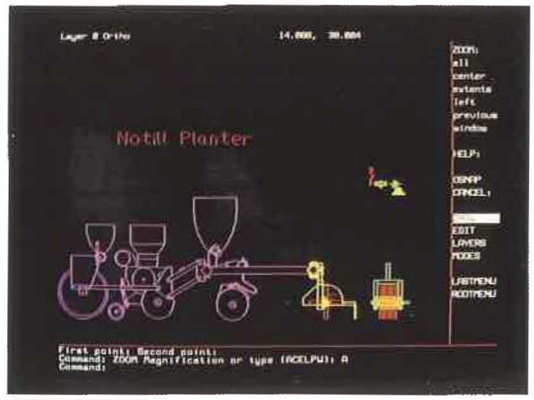


Part of the research laboratories of the St. Anthony Falls Hydraulic Laboratory. Research workers at the Laboratory have developed expertise in scientific computing in many areas of fluid mechanics.

St. Anthony Falls Hydraulic Laboratory

The St. Anthony Falls Hydraulic Laboratory is a unique research facility located at the head of St. Anthony Falls on the upper Mississippi River as it flows through downtown Minneapolis. Water passes through the facility and back to the river below the Falls after serving as the means to conduct a variety of experimental studies in hydraulics and related fields. For nearly 50 years, fundamental research in fluid mechanics as well as applied research in the design and analysis of hydraulic structures and special apparatus and equipment has been conducted here, helping the Laboratory gain an international reputation.

Recently, St. Anthony Falls researchers have used supercomputers to overcome some of the tremendous challenges of fluid mechanics. Examples include studies of flow modeling for wind tunnels conducted by Professor Cesar Farell; simulation of viscous flow with flow separation and large eddies by Professor Charles Song; and modeling of the transient convection by heat loss in lakes by Professor Heinz Stefan.



Economics and Management

Like many of the physical sciences, economics and management theory are confronted by systems of tremendous complexity. Not only do the economies of nations pose vast mathematical challenges, but such smaller scale issues as inventory control and production scheduling often require the most advanced computing technology available.

Because of the resources of the Minnesota Supercomputer Institute, members of the University of Minnesota School of Management now have several years of experience using supercomputers to simulate economic systems and management and manufacturing operations. Professor Chris Sims, for instance, uses a Cray machine to do macro-economic modeling for the Ninth Federal Reserve District, headquartered in Minneapolis. Sims and other Minnesota researchers have also created the largest macro-economic models yet attempted of the U.S., Europe and Japan as similar and linked economic systems that interact through financial markets, imports and exports. Work began using a Cray 1, but the size of the model and the new estimation techniques it uses required that it be transferred to the giant memory of the Cray 2.

Agriculture

Supercomputers can also aid in the study of agricultural economics. Supercomputer simulation can provide information on the most effective ways to manage flocks and herds. One Minnesota researcher has already used five hours on a Cray machine to model optimal methods of poultry production, an important Minnesota industry.

Since many other areas related to agriculture require sophisticated computer analysis, efforts are underway at Minnesota to develop vectorized finite and boundary element codes for agricultural supercomputer applications. For example, supercomputers will allow researchers to model the processes associated with the cracking of soil during dessication, or simulate the movement of moisture and chemicals through the layers of earth above aquifers. Supercomputers can also be used to model agricultural equipment and machinery. Some of this work has been done with conventional computers, but when finite element analysis and real-time simulation are required, supercomputing will provide benefits to agricultural engineering that it is now providing to so many other areas.

Some of the Fellows of the Minnesota Supercomputer Institute and their colleagues and students. The program developed from modest scale support of scientific research on the University's Cray 1 in 1981, to a program of national stature that today involves over 200 University faculty members and students.

Design and Typography: Larsen Design Office, Inc.
Writing: George Dixon
Photography: Paul Shambroom
Printing: Litho Specialties, Inc.

MINNESOTA

SUPERCOMPUTER

INSTITUTE

1200 WASHINGTON

AVENUE SOUTH

MINNEAPOLIS

MINNESOTA

5 5 4 1 5