PROPOSAL

A Center for Scientific and Engineering Supercomputing



University of Illinois at Urbana-Champaign

PROPOSAL

A Center for Scientific and Engineering Supercomputing

Larry Smarr - Astronomy
John Kogut - Physics
David Kuck - Computer Science
Robert Wilhelmson - Atmospheric Sciences
Peter Wolynes - Chemistry
Karl Hess - Electrical Engineering
Thomas Hanratty - Chemical Engineering
Robert McMeeking - Theoretical and Applied Mechanics

PROPOSAL TO THE NATIONAL SCIENCE FOUNDATION
Cover Page

FOR CONSIDERATION BY NSF ORGANIZATIONAL UNIT (Indicate the most specific unit known, i.e. program, division, etc.)	IS THIS PROPOSAL BEING SUBMITTED TO ANOTHER FEDERAL AGENCY? Yes ____ No X ; IF YES, LIST ACRONYM(S):
Edward R. Knapp Director of National Science Foundation	

PROGRAM ANNOUNCEMENT/SOLICITATION NO.:	CLOSING DATE (IF ANY):

NAME OF SUBMITTING ORGANIZATION TO WHICH AWARD SHOULD BE MADE (INCLUDE BRANCH/CAMPUS/OTHER COMPONENTS)

Board of Trustees
University of Illinois at Urbana-Champaign

ADDRESS OF ORGANIZATION (INCLUDE ZIP CODE)

506 South Wright Street
Urbana, IL 61801

TITLE OF PROPOSED PROJECT

A Center for Scientific and Engineering Supercomputing

REQUESTED AMOUNT	PROPOSED DURATION	DESIRED STARTING DATE
$42,751,000.00	5 years	April 2, 1984

PI/PD NAME	PI/PD PHONE NO.
Larry L. Smarr [redacted]	[redacted]

PI/PD DEPARTMENT	PI/PD ORGANIZATION
Department of Astronomy	University of Illinois

ADDITIONAL PI/PD AND SSN*	ADDITIONAL PI/PD AND SSN*
ADDITIONAL PI/PD AND SSN*	ADDITIONAL PI/PD AND SSN*

FOR RENEWAL OR CONTINUING AWARD REQUEST, LIST PREVIOUS AWARD NO.:	SUBMITTING ORGANIZATION IS ____ IS NOT ____ A SMALL BUSINESS CONCERN (see CFR Title 13, Part 121 for definitions).

*Submission of social security numbers is voluntary and will not affect the organization's eligibility for an award. However, they are an integral part of the NSF information system and assist in processing the proposal. SSN solicited under NSF Act of 1950, as amended.

CHECK APPROPRIATE BOX(ES) IF THIS PROPOSAL INCLUDES ANY OF THE ITEMS LISTED BELOW:

- ☐ Animal Welfare
- ☐ Human Subjects
- ☐ National Environmental Policy Act
- ☐ Endangered Species
- ☐ Marine Mammal Protection
- ☐ Research Involving Recombinant DNA Molecules
- ☐ Historical Sites
- ☐ Pollution Control
- ☐ Proprietary and Privileged Information

PRINCIPAL INVESTIGATOR/ PROJECT DIRECTOR	AUTHORIZED ORGANIZATIONAL REP.	OTHER ENDORSEMENT (optional)
NAME Larry L. Smarr	NAME Linda S. Wilson	NAME J. J. Kamerer
SIGNATURE	SIGNATURE	SIGNATURE
TITLE Associate Professor	TITLE Secretary Campus Research Board	TITLE Director Grant & Contract Admin.
DATE	DATE	DATE

TABLE OF CONTENTS

I. Statement of Purpose

II. The Need for Supercomputers in American Universities

III. The Center for Scientific and Engineering Supercomputing

A. The Nature of the Center

B. The Management of the Center

C. The Future of the Center

IV. Scientific and Engineering Research Program

V. The Integrated System Configuration

A. Principles of a Well-Balanced System

B. Selection of a Supercomputer

C. Distributed Network

D. Staffing

VI. Budget and Timetable

VII. Appendices

A. Group I Users

B. Group II Users

C. Historical Sketch of Supercomputing at Illinois and Current Campus Computing

D. Vita's of the Principal Investigators

NOTICE OF RESEARCH PROJECT

SCIENCE INFORMATION EXCHANGE

SMITHSONIAN INSTITUTION
NATIONAL SCIENCE FOUNDATION

PROJECT SUMMARY

SIE PROJECT NO.
NSF AWARD NO.

FOR NSF USE ONLY			
DIRECTORATE/DIVISION	PROGRAM OR SECTION	PROPOSAL NO.	F.Y.

NAME OF INSTITUTION (INCLUDE BRANCH/CAMPUS AND SCHOOL OR DIVISION)

University of Illinois at Urbana-Champaign

ADDRESS (INCLUDE DEPARTMENT)

Board of Trustees
506 South Wright Street, Urbana, IL 61801
(for the Departments of Astronomy, Physics, Computer Science, Atmospheric Sciences, Chemistry, Electrical Engineering, Chemical Engineering, Theoretical and Applied Mechanics)

PRINCIPAL INVESTIGATOR(S)

Larry L. Smarr, John Kogut, David Kuck, Robert Wilhelmson, Peter Wolynes, Karl Hess, Thomas Hanratty, Robert McMeeking

TITLE OF PROJECT

A Center for Scientific and Engineering Supercomputing

TECHNICAL ABSTRACT (LIMIT TO 22 PICA OR 18 ELITE TYPEWRITTEN LINES)

Several orders of magnitude improvement in computer power is urgently needed in American Universities. As a first step, we propose the creation of a Center for Scientific and Engineering Supercomputing at the University of Illinois. The Center is meant to be a model of a new type of dedicated basic research facility in which large-scale problems of heretofore intractable complexity, in a wide variety of disciplines, can be successfully attacked. The Center will provide a focal point for bringing together innovative scientists, engineers, computer designers, and algorithm developers. They will work in a fully equipped, well balanced facility consisting of a supercomputer, a high speed communications network, a mass storage system, a central output facility, local nodes for pre- and post-processing and display of data, and an adequate staff. The Center will serve selected University of Illinois research programs and the national community. The majority of the time will be allocated by an external program committee, who will consider requests from any investigator, regardless of his university affiliation. Excellence, as determined by peer review will be the criterion for determining access to the Center. The University of Illinois is well prepared to provide the leadership needed for this new initiative as it combines a long tradition of supercomputer design with a broadly based high quality scientific and engineering research program. We believe that the proposed Center will have a dramatic impact on basic research in the United States.

1. Proposal Folder
2. Program Suspense
3. Division of Grants & Contracts
4. Science Information Exchange
5. Principal Investigator
6. Off. of Govt. & Pub. Progs.

I. STATEMENT OF PURPOSE

Several orders of magnitude improvement in computer power is urgently needed in American universities. As a step toward that goal, we propose the creation of a Center for Scientific and Engineering Supercomputing at the University of Illinois. The Center is meant to be a model of a new type of dedicated basic research facility in which large-scale problems of heretofore intractable complexity, in a wide variety of disciplines, can be successfully attacked. The Center will provide a focal point for bringing together innovative scientists, engineers, computer designers, and algorithm developers. They will work in a fully equipped, well balanced facility. The facility will be modeled on the highly successful ones at the national laboratories. The Center will serve selected University of Illinois research programs and the national community. The majority of the time will be allocated by an external program committee. Excellence, as determined by peer review will be the criterion for determining access to the Center. The interaction of these talented users, combined with unprecedented amounts of computational resources per investigator, should lead to major advances in a number of frontier research areas.

To demonstrate the amount of local need, we have identified and documented 17 major basic research programs in science and engineering at the University of Illinois which will benefit immediately from access to the proposed Center. A number of these programs currently use remote supercomputers. These programs involve approximately 25 professors at Illinois, 92 graduate students, and 61 off-campus collaborators. Astrophysics, elementary particle physics, materials research, quantum chemistry, atmospheric sciences, supercomputer architecture and algorithms, and electrical, chemical, and mechanical engineering are represented. In addition, another 50 Illinois professors, along with their graduate students and off-campus collaborators, have documented their need for a large increase in computational capacity. Local and external users will saturate a supercomputer with first-rate basic research in about two to three years.

Although single processor speeds are continuing to grow, the problems of interest have grown much more rapidly. To try and bridge this gap, it is almost universally agreed that future increases in supercomputer speed will have to come from employing multiple processors, along with enormously increased memory sizes. Our proposed supercomputer will combine multiprocessor technology with high speed vector pipeline architecture and a hierarchical memory structure. This will challenge users to learn to program on multiprocessors and computer scientists to develop new compilers, algorithms, and languages to use efficiently this new generation of computers. The Laboratory for Advanced Supercomputers at the University of Illinois is one of the leading research groups in multiprocessors, vectorization, and memory hierarchies. Its members will be intimately involved in the Center's work. We expect that our experience will provide vital feedback to commercial computer vendors, to the national laboratories, and to other supercomputer users.

The University of Illinois is well prepared to provide the leadership needed for this new initiative. The University combines a long tradition of supercomputer design with a broadly based high quality scientific and engineering research program. This is underscored by the fact that this proposal emanates from the scientists and engineers at the university. Furthermore, our University has a proven record of encouraging and managing major new computational research programs. By creating a Center for Scientific and Engineering Supercomputing in such a fertile environment, we intend to establish a model for the development of similar Centers at other major universities in the near future.

The plan presented below is very aggressive in its scientific content and the technology applied to its pursuit. It is quite conservative in its method of introducing that technology, operating with proven equipment, an initial selection of already running software, and a facilities management plan growing out of the well established capabilities and philosophies of the national laboratories. We believe that the proposed Center will have a dramatic impact on basic research in the United States.

II. THE NEED FOR SUPERCOMPUTERS IN AMERICAN UNIVERSITIES

In a number of disciplines, some of the brightest and most innovative people are discovering that large-scale computer simulations are an indispensable tool. These disciplines include the diverse fields of astrophysics, high energy and many-body physics, materials and biomolecular research, atmospheric sciences, computer-aided-design, structural analysis, computer science, and turbulence. The use of the largest and fastest computers, termed supercomputers, to explore the basic laws of nature in dynamic and physically complex regimes, or to simulate complex engineering structures, is leading to many new insights.

To illustrate the kind of problem in which the supercomputer is the *sine qua non* , we summarize three examples of work done by Illinois researchers. The calculation of the head-on collision of two black holes by Eppley and Smarr demonstrated that the full Einstein equations could be solved in time dependent, multidimensional, strong field regimes. They found that black holes were stable to very large deformations and demonstrated that the linearized concept of "ringing modes of black holes" which generate gravitational radiation, carried over to the full theory. In gauge theories of elementary particle physics, computer simulations have provided the first theoretical evidence for quark confinement and dynamical mass generation. Numerical simulations run by Kogut, Stone and Wyld are influencing high energy experimental programs and should play an important role in the planning of a U.S. heavy-ion accelerator. Storm research has been significantly enhanced through three-dimensional modeling of cloud evolution and internal structure. Tornadic storms have been simulated by Wilhelmson and collaborators and successfully combined with observational data to study how these storms move and develop strong internal rotation.

This kind of scientific revolution was clearly forecast over 30 years ago by John von Neumann. The eminent mathematician Garrett Birkhoff makes this point strongly in a recent review article titled "Numerical Fluid Dynamics". He paraphrases John von Neumann's vision as follows:

> "It seems clear...that von Neumann was envisioning fluid dynamics as a *mathematical science* as had Euler, Lagrange, Stokes, Riemann, and Poincare before him. His main point was that mathematicians had nearly exhausted *analytical* methods, which apply mainly to *linear* DE's and *special geometries*... In short, von Neumann's proposal was that, with high speed digital computers, one could substitute *numerical* for analytical methods, tackling *nonlinear* problems in *general* geometries."
>
> - SIAM Review *25* , 1 (1983)

Birkhoff notes that since von Neumann made these remarks, computing machines have increased in speed by one billion and become cheaper per computation by a factor of ten million. Assessing where we are today, Birkhoff concludes that:

> " ...numerical fluid mechanics has not and will not replace either analytical or experimental fluid mechanics as a research tool, but that it complements and supplements them invaluably."
>
> - op. cit.

Extending this lesson to a general conclusion, mathematician James Glimm of the Courant Institute of Mathematical Sciences (and former chairman of the NSF Advisory Committee in Mathematics) recently wrote:

> "Computers will affect science and technology at least as profoundly as did the invention of calculus. The reasons are the same. As with calculus, computers have increased and will increase enormously the range of solvable problems. The full development of these events will occupy decades and the rapid progress which we see currently is a strong sign that the impact of computing will be much greater in the future than it is today."
>
> *-Frontiers of Supercomputing* , proceedings of the conference at Los Alamos, August, 1983.

The style of research which brings physicists and mathematicians together to attack unsolved problems is much older than computing machines. In this century it was embodied in the Gottingen School (Klein, Minkowski, Hilbert, Courant, Runge-Kutta, Born, Heisenberg, Prandtl, etc.). This spirit was transported to America in the 1930's and set up in the Courant Institute of Mathematical Sciences at New York University. Out of this approach has come much of modern mathematics and theoretical physics. Unfortunately, since the mid-1960's in the United States, the Gottingen-Courant-von Neumann style, coupled with digital computers, has been primarily directed toward mission-oriented efforts in national centers (e.g. nuclear weapons development, weather forecasting, aerodynamics design, and fusion energy research) or industrial laboratories. Although this development has shown the true power of computers to attack complex physical and engineering systems, it has remained largely separated from the mainstream of basic research in American universities.

As a result of this history, the current distribution of supercomputers today virtually excludes American universities. As of mid-1983 there are approximately 75 supercomputers in the world (Table 1), these being either the CRAY-1 made by Cray Research or the Cyber 205 made by Control Data Corporation. In this country the national DOE weapons labs have the largest concentrations of them. Los Alamos National Laboratory (LANL) and Lawrence Livermore National Laboratory (LLNL) together have ten CRAY's. Specialized scientific disciplines have access at National Centers to CRAY's, [e.g. the National Center for Atmospheric Research (NCAR), the National Magnetic Fusion Energy Computing Center (NMFECC), and the National Aeronautics and Space Administration at Ames] or Cyber 205's, [e.g. Geophysical Fluid Dynamics Laboratory (GFDL)]. Finally a number of major corporations have acquired supercomputers for their industrial research laboratories, e.g. Bell Labs and Exxon. European scientific centers have also begun using supercomputers , e.g. the Max-Planck Institute (MPI) for Physics and Astrophysics in Garching-bei-Munchen, West Germany. Most of these facilities are fully equipped with adequate peripherals (disks, mass store, printers, graphics, etc.) for post-processing the prodigious output of a supercomputer.

The first arrival of supercomputers at American universities has occurred only recently. Colorado State University and Purdue University have each bought a Cyber-205, while the University of Minnesota has obtained a CRAY-1. Although this is a welcome development, these facilities have had less immediate impact than they might have had, because the researcher must obtain a grant for the very high cost of the computer time. For instance, time for outside users on the CRAY-1 at Minnesota or the Cyber 205 at Colorado State is approximately $1000-$2000/CPU hour, while the financially more accessible system at Purdue is just going into production. It is clear that a significant research program requiring 200 hours per year, for example, is prohibitively expensive for scientists with NSF funding. In addition, these universities do not have enough peripherals to fully utilize these machines or to run them interactively. The result is that many scientists and engineers simply avoid undertaking research requiring supercomputers. This situation should not be taken as representing a limitation of university capability, but rather of the financial requirements to effectively enter the supercomputer business. The real test of university supercomputers will come in several years after an adequate configuration is available, an adequate staff is assembled, a community of users has grown active, and the difficult period of assimilation has passed. This proposal is aimed directly at achieving success in that context.

TABLE 1

WORLD CENSUS* OF SUPERCOMPUTERS

Country	Site	Number	Purpose	Computer
U.S.	Los Alamos Nat. Lab.	5	Weapons Research	Cray-1
	Lawrence Livermore Nat. Lab	4 2	Weapons Research Magnetic Fusion Energy Research	Cray-1
	Sandia Nat. Lab	2	Weapons Research	Cray-1
	KAPL	1	Reactor Research	Cyber 205
	Bettis	1	Reactor Research	Cyber 205
	Kirtland Air Force Base	1	Military	Cray-1
	National Center for Atmospheric Research	1	Atmospheric Science	Cray-1
	NSA	2	Intelligence	Cray-1
	NASA-Ames	1	Aerodynamics	Cray-1
	NASA-Goddard	1	Atmospheric Science	Cyber 205
	NASA-Lewis	1	Fluid Dynamics	Cray-1
	FNOC-Monterey	1	Oceanography	Cyber 205
	National Environmental Satellite Service (NOAA)	1	Research	Cyber 205
	Geophysical Fluid Dynamics Laboratory	2	Geophysical Research	Cyber 205
	Colorado State Univ.	1	Engineering Research	Cyber 205
	Univ. of Minnesota	1	Research	Cray-1
	Purdue University	1	Research	Cyber 205
	Bell Labs	1	Research	Cray-1
	ARCO	1	Petroleum Engineering	Cray-1
	EXXON	1	Petroleum Engineering	Cray-1
	CHEVRON	1	Petroleum	Cray-1
	TEXACO	1	Petroleum Engineering	Cyber 205
	SOHIO	1	Petroleum Engineering	Cyber 205
	Grumman Corp.	1	Jet Engine Simulation	Cray-1
	Westinghouse Corp.	1	Nuclear Power Plant Design	Cray-1
	Digital Production Inc.	1	Graphics	Cray-1
	Boeing Computing Serv.	1	Timesharing	Cray-1
	Control Data Corp.	1	Timesharing	Cyber 205
	United Information Serv.	1	Timesharing	Cray-1
Germany	Max Planck	1	Research	Cray-1
	Bochum	1	Research	Cyber 205
	PRAKLA	1	Research	Cyber 205
	Univ. of Karlsruhe	1	Research	Cyber 205
	Univ. of Stuttgart	1	Research	Cray-1
	Deutch Forschungs und Versuchsanstalt fur Luft Raumfahrt	1	Aerospace Research	Cray-1
France	GETIA	1	Electric Power Institute	Cray-1
	Commissariat A'Lenergie Atomique	1	Nuclear Energy	Cray-1
	Compagnie International De Services En Informatique	1	Timesharing	Cray-1
	Ecole Polytechnique	1	Research	Cray-1

England	European Centre for Medium Range Forecasting	1	Weather	Cray-1
	Brit Met	1	Weather	Cyber 205
	Daresbury	1	Physics Research	Cray-1
	AWRE Harwell	1	Nuclear Energ, Weapons	Cray-1
	Shell Oil, U.K.	1	Petroleum	Cray-1
	Univ. of London	1	Research	Cray-1
	Univ. of Manchester	1	Research	Cyber 205
Japan	Mitsubishi	1	Research	Cray-1
	Century Research	1	Research	Cray-1

* Taken from the Lax "Report on Large Scale Computing in Science and Engineering" (Dec. 26, 1982).

The computing power drought in American universities over the last five years has resulted in a drain of highly talented researchers from the universities to sites with fully equipped supercomputer systems. There have been two major stages in this process: first, a flight to the weapons labs (LLNL and LANL) or to industry, and second, a flight to foreign computing centers. This process is not only depleting American universities of faculty doing important research, but has also made it difficult to train future researchers in the use of supercomputers. The shortage of new scientists and engineers competent in fields requiring numerical research is becoming critical.

This critical problem can be illustrated by examining the development of computational astrophysics during the last decade. Areas of numerical research include: supernovae, black holes, neutron stars, gravitational waves, cosmology, pulsating stars, accretion onto compact objects, jet formation, star formation, and radiation astrophysics. Many scientists from academia who wanted to work in these frontier fields have had no choice but to go to the national labs (LLNL and LANL primarily) to gain access to the state of the art computers. As a result of this limited access, as well as the standard shortcomings of American universities (i.e. low salaries, lack of job openings, etc.), many of these people have permanently left the universities to become lab employees.

More recently, computational astrophysicists have been going to the Max-Planck Institute of Physics and Astrophysics (MPI) in Munich, West Germany to do their computing. This is because the MPI CRAY-1 is part of a research institute devoted to *basic research* in physics, astrophysics, chemistry and plasma physics, not to mission-oriented applied research. Even scientists employed at our national DOE weapons laboratories can sometimes get more CRAY time for their astrophysics projects at MPI than they can internally at LLNL or LANL. There are about 100 visitors to MPI per year, of which approximately 20 are heavy CRAY users. Although MPI is a model for what is needed in the United States, it is grossly underconfigured by the standards of our national laboratories.

While America is suffering the loss of faculty members, foreign researchers are becoming strongly competitive with American programs. For example, the Japanese have major astrophysics research programs which utilize numerical hydrodynamics. Topics include study of protostars, stellar evolution, accretion onto compact objects, radio jets, general relativity, and cosmology. Although currently they are limited by their available computers, starting this Fall 1983, Japanese supercomputers (e.g. Hitachi S810-20 and Fujitsu VP-200), as powerful as the new CRAY X-MP or Cyber 205, will begin to be placed in Japanese universities. At that point it is highly likely that Japan and Germany (receiving a CRAY X-MP this fall) will rapidly begin to take over the scientific leadership in numerical astrophysics from American universities, unless drastic action is taken in the United States.

This story can be repeated for many of the major fields of scientific and engineering research. For example, large scale computer simulations in relativistic quantum field theory and high energy physics, which were pioneered in this country, are now being carried out almost exclusively in Europe and Japan. Several CRAY-1 and Distributed Array Processors (ICL-DAP) in Britain are dedicated to theoretical physics. In Germany, a Cyber 205 at Bochum University is available to physicists doing pioneering lattice gauge theory simulations of the strong interactions. In France, several new CRAY-1 systems have been installed recently at Ecole Polytechnique and various campuses of the University of Paris. In fact, European Institutes have become one of the largest markets for supercomputer systems over the past year. Since theoretical physicists in the United States have severely limited access to comparable facilities, their eminent position in these fields is in serious jeopardy.

To meet this challenge it is clear that a new type of research facility is needed in American universities. Only in this manner will we be able to rejoin this exploding area of basic research. This facility must be at the state of the art in both its supercomputer and its associated support equipment, so as to take full advantage of the computational speed. Using this new tool as a magnet, the facility must then encourage the top minds in computer architecture and algorithm development to interact constantly with creative scientists and engineers so that new techniques for attacking previously intractable problems can be developed and utilized.

Today there is no fully equipped supercomputer facility in the U.S. dedicated to basic research in all fields of science, engineering and scholarship. On the one hand, research facilities which bring together scientists with a range of interests (Princeton Institute for Advanced Study, Santa Barbara Institute for Theoretical Physics) have no major research equipment. On the other hand, facilities which contain other types of expensive research instruments (telescopes, particle accelerators, laser laboratories) each serve only a narrow speciality. In contrast, the supercomputer has the potential to be a widely applicable tool, which can have impact on myriad specialities. Thus, in a number of ways the new type of supercomputer facility we envision would be unique and could serve as a new model for large areas of scientific and engineering research in America.

It is often argued that the supercomputer crisis could be met by placing a few more in national laboratories, and allowing all scientists and engineers in American universities who need a supercomputer to access the machine remotely. Indeed the models for this, NCAR and NMFECC, are very successful. However, these facilities serve specific disciplines (Atmospheric Sciences and Magnetic Fusion) whose practitioners already interact scientifically.

In contrast, major university programs, centered around local systems, would enable otherwise isolated remote users from many fields to share and learn from one another. This will encourage cross-disciplinary interaction which is quite unlikely to occur when a site is remotely located. In addition, a local supercomputer will have a very strong impact on graduate student training.

Furthermore, at a few universities, such as Illinois, researchers already use about 850 hours/year of supercomputer time remotely (see Section IV for details). If a new facility is to have a major impact on their work, thus avoiding the failure of the National Resource for Computational Chemistry, an order of magnitude more time must be made available. Because the user base identified in this proposal can saturate a supercomputer, the only economical solution is to place it locally.

While the DOE has made important strides to provide more remote supercomputer time to university researchers in recent years, many still have large unmet needs. For example, in our Physics Department John Kogut and his group, working on lattice gauge theory, have been able to obtain some 50 CRAY 1-A hours per year at LANL and NMFECC. However, their scientific needs have far exceeded this amount. In addition, most of the computer time obtained required a visit rather than true remote computing. (See Appendix A). The theoretical physics community, responding to a DOE initiative in 1983, requested 1100 CRAY hours be made available for their computations. DOE was able to respond with a new allocation of 60 hours on the MFE machine; the Illinois group got 8 hours which translated into 24 minutes per week over the remainder of the fiscal year. Obviously this allocation, which was obtained after much delay and time-consuming work on proposals, is of very limited use. Similar restrictions (limited time and funding for university-based users) on the open CRAY-1 at Los Alamos have limited its impact on university researchers as well. While the DOE as well as the national laboratories have further plans to increase computing power and availability, it seems clear that the national computing environment cannot be significantly improved unless more supercomputer power can be concentrated in the hands of large users.

We do believe that several remote supercomputers should be made available nationwide to serve researchers in universities which can not provide enough demand to justify a local supercomputer. Nonetheless, a real breakthrough in this scientific revolution will only occur when integrated supercomputer facilities, representing the state of the art, are placed in a number of selected American universities with strong graduate research programs in science and engineering.

III. THE CENTER FOR SCIENTIFIC AND ENGINEERING SUPERCOMPUTING

III.A. The Nature of the Center

The University of Illinois is prepared to make a dramatic and decisive move toward realizing a major breakthrough in computing in American universities. We propose to create a Center for Scientific and Engineering Supercomputing which will bring together, in a university setting, many of the world's best scientists, engineers, computer designers, and computational algorithm developers. They will have at their disposal the best computational facility current technology allows. They will interact in seminars and in their work, sharing expertise and insights. Out of this mix at the Center we fully expect 1) major breakthroughs in scientific and engineering problems; 2) new computer algorithms, software, designs, and theory; 3) to train a whole generation of researchers and graduate students and 4) to gain experience in setting up such centers.

We propose to bring to the Center the most advanced supercomputer that is readily usable by scientific and engineering researchers. This supercomputer should have extremely fast processing capabilities over a wide range of applications, while maintaining compatibility with a mature and widely-used software base. For the supercomputer to be productive, it must be part of a fully integrated system, a detailed description of which is given in Section V. It must have adequate mass storage, graphics, and hard copy facilities, as well as a high speed smart-terminal network. Our criterion for "adequate" is that the turnaround time for any phase of the computation process should be so short that it does not discourage the progress of a creative scientist or engineer.

Currently, only national laboratories possess such integrated supercomputer systems. We have visited most of the major national supercomputer laboratories (LLNL, LANL, NMFECC, NCAR, GFDL) to determine what is needed to equip and staff such a facility. We will model our Center's system on the best components from these laboratories, with close cooperation with their staff. In this way, we can share the enormous experience (many man-centuries) which the laboratories have gained in operating systems, hardware configurations, and software utilities, as well as in facilities management. Our Center will be a dedicated *basic research facility* used intensively to solve scientific and engineering research problems done best on a supercomputer.

We anticipate that the supercomputer will be used continuously by about 25-50 collaborative groups at the University (Appendices A and B; Section IV). For each Illinois professor in these research groups, there are on average two off-campus collaborators and three graduate students who will also be active users of the facility. Thus, the potential user group is estimated at around 300-400 scientists and engineers. Because of the relatively small number of investigators using our facility, we estimate that an individual researcher will have up to ten times the computer power than he currently can obtain elsewhere. This will allow the Center to encourage breakthrough calculations. The solution of such problems should stimulate much new theoretical, observational, and experimental work. Thus, we can view such a facility as a new engine for scientific and engineering progress.

In addition to providing access to about one hundred off-campus collaborators, the University of Illinois will fund a Visitors Program, administered by a Program Committee of eminent scientists and engineers, most of whom will not be affiliated with the University of Illinois. The Visitors Program will bring to the Center world leaders in applying supercomputers to frontier fields and allow them to use a portion of the Center's supercomputer time. We will devote about 25% of the machine in the first year of full scale operation (approximately 3000 CRAY-1 equivalent hours) to the Visitors Program.

We propose that the Illinois Center be fully funded, so that neither internal nor external users will require often unobtainable grant funds to obtain large blocks of time on the supercomputer. Excellence, as determined from peer review by an Internal Allocation Board and an outside Program Committee, will be the only criterion for access. We believe this approach will lead to significant acceleration in the pace of research in scientific and engineering supercomputing. This approach is also followed at NCAR, NMFECC, and MPI. All of these institutes have first class research programs.

It must be relatively easy for the user to take advantage of the machine's architecture. A particularly exciting feature of the Center will be the direct interaction between these users and the Laboratory for Advanced Supercomputers (LAS) in the Department of Computer Science at Illinois. The Laboratory is one of the world's leading groups in designing the system software and numerical algorithms for efficient use of advanced architectures. They have devised an advanced code optimizer (Parafrase), to vectorize sequential programs, that explicitly pinpoints programming which requires further work. This interaction will be invaluable for users, particularly those without extensive experience in vectorization, helping them make the most efficient use of their time. The Laboratory is also developing methods to use multiprocessors effectively for a single computer program; a boon for the user of the new generation of multiprocessors.

The Laboratory is also very active in the design of supercomputers, having had direct or indirect influence on many industrial developments in the past decade. This group has recently announced that they are beginning to develop the Cedar multiprocessor system. The goal of the Cedar Project is to produce a gigaflop (one billion floating point operations per second) machine in the next few years. This effort will have two fruitful interactions with the Center. First, the LAS will be a user of a good deal of supercomputer time in the design and simulation of the Cedar hardware and software. Second, it will take advantage of the Center's user community to collect algorithms and programs that typify user requirements, in an effort to make the Cedar system responsive to future needs. Closing the feedback loop from users to designers is extremely important and seldom done in as direct a way as will be possible by having these activities co-located at Illinois.

Because the Center is set in a large research university, a rich diversity of fields will be exposed to the exciting capabilities of large scale computing. We expect that this will create a number of novel uses for supercomputers in virgin fields. Having graduate students active in all phases of the Center's work may produce the biggest payoff. Bright, talented, young students can often see innovative new approaches more easily than their elders. Furthermore, their training will spread these new techniques to other universities, industry and national laboratories.

This point has been emphasized in the 1982 Lax Report on "Large Scale Computing in Science and Engineering."

> "Another important component of this National Program is the development of an imaginative and skilled user community in supercomputing. There is a considerable shortage of appropriately trained personnel and of training opportunities in this area. Forms of institutional encouragement, such as NASA's special fellowships in the area of numerical fluid mechanics, special summer schools, and special allocation of access time to supercomputers for those projects that involve graduate students, should be considered. Some of the more mathematical aspects of these activities can be accomplished independently of the machines on which the actual calculations are done; however, the true integration of methods and their implementation cannot be done without access to supercomputers. The nature of the machine architecture has a very profound effect on the numerical methods, on the algorithms, and of course on the software. Thus, while being trained, students must have access to state of the art computers. Today such training is virtually nonexistent; yet the skills gained from such training are essential to science and engineering."
>
> -Lax Report, p. 12-13

Cross-disciplinary sharing will also be fostered by the common computing facility. For instance, at Illinois in the last year, there has been a very valuable interaction between Computational Astrophysicists and Atmospheric Scientists. This includes areas of finite differencing, graphical representation of solutions, physics of hydrodynamics, and image processing techniques. This interaction was brought about because a shared computing facility (partially supported by the NSF), the VAX and Image Processing Center, was developed by the two departments and the Computing Services Office. This facility brought these two groups of scientists together for the first time, even though their Departments are located in adjacent buildings! Our Center will create many more opportunities for sharing across disciplines.

To help spread knowledge about supercomputing, we plan to have weekly colloquia in which local researchers and our Visitors give talks on their work. Annual conferences on various aspects of supercomputing will also be sponsored. This will provide an opportunity for scientists and engineers from many disciplines to come together to discuss their common tool, the supercomputer. We also plan to organize a Summer Supercomputing Program since many more visitors will be able to come to Urbana during the summer.

The impact on American industry will also be great. We hope to have industrial researchers come to the Center to share with us their vision of where the computational frontiers are. This crucial interaction was underscored by the National Science Foundation's Press Report "Prospectus for Computational Physics" [Report by the Subcommittee on Computational Facilities for Theoretical Research to the Advisory Committee for Physics, Division of Physics, March 15, 1981]:

> "Students trained by university physicists move into positions in national laboratories and industry, bringing with them the training in the present state of the art in tackling the complexity of problems being simulated. A number of the problems now being studied in industry are challenging and broad enough to be legitimate subjects for basic research; industrial workers in these problems should be integrating themselves into the basic research community through exchange of seminar speakers, publication in common journals, etc., as well as being integrated at some level into a computational physics network."
>
> -Press Report, p. 22

Our graduate students in Computer Science are already having a major impact on industry, for example in the design of the next generation of supercomputers. Steve Chen, designer of the new CRAY X-MP supercomputer, was a Ph.D. student in computer architecture under Professor Dave Kuck, a Principal Investigator on this proposal. That computer is now a prime candidate for our Center. Such interaction between universities and industry will help both corporate computer consumers and producers. This is rare at the present time, which is one of the key reasons that the United States is being successfully challenged by the Japanese in the supercomputer market.

III.B The Management of the Center

We now turn to the details of the governing structure of the Center. Our primary objective in designing this governance hierarchy is to maximize the productivity of our scientific and engineering users. This will require that these users will be involved in many areas of management at the Center. On the other hand, we do not want to waste their time on the implementation of policy in highly technical areas of hardware and software. Therefore we will have the highest quality professional staff to help in the formulation of policy and to carry that policy out efficiently. We will draw on expert outsiders for oversight committees in both research and management.

The Center will be operated as a dedicated research facility separated from the normal campus computer activity. To assure that we can provide access regardless of speciality, the Center will be administratively located in the Graduate College. Its financial and computer management will be integrated into the Computing Services Office (CSO).

We now define and explain the five major parts of the management structure we propose: a Program Committee, a Scientific Director, a Policy Board, the Internal Allocation Board, and a Facilities Management Advisory Board.

The *Program Committee* will be a panel of eminent scientists and engineers mostly from institutions other than the University of Illinois. The members will be selected in careful consultation with NSF staff to provide broad disciplinary, regional, and institutional representation. The Program Committee has four major areas of responsibility. The first requires the Committee to oversee the Visitor Program, which will bring in some of the world's most innovative computational scientists for extended stays to do their own research. Nominations for the Visitor program will be forwarded to the Program Committee by University

of Illinois Departments, as well as by anyone desiring to be a visitor to the Center. This will assure equitable access to outside users. The University of Illinois will contribute toward the Visitors Program at a level of about $200,000 per year. Second, the Committee will allocate the majority of the computer time, through peer review of proposals. These proposals can come from any investigator, regardless of affiliation. Third, the Program Committee will periodically review the decisions of the Internal Allocation Board to insure a high quality of internal scientific research at the Center. Fourth, the Committee will provide advice and guidance to the Scientific Director. We expect that during the next few years, a number of other Centers will be situated at universities or national laboratories. Our Visitor Program will be a valuable training ground for building a user base for these other machines as well as having an immediate impact on major scientific breakthrough projects.

The *Scientific Director* for the first several years will be the lead Principal Investigator on this proposal, Larry Smarr. He has had eight years of working experience in supercomputing facilities (LLNL and MPI) as well as several years advising the NSF on supercomputers (Press, Lax, and Curtis Reports). He will be released from teaching and committee duties by his Departments and will divide his time between his own research program described in Appendix A and the Scientific Director's duties. After the Center is well started, this position will be filled by a national search for a permanent Director. The salary of the Director will be contributed by the University of Illinois. The main job of the Scientific Director is coordinating all the aspects of the Center's activities to assure the maximum possible research output. He will work with the Policy Board on establishment of policy and objectives, and then with the management and staff to carry these out. He will also take part in the annual salary and promotion review for the technical staff. He will not be directly involved in the time allocation on the supercomputer. We believe it is important that the Director be a person who has both considerable experience in supercomputer laboratories and is also an active user of the proposed Center itself. The Director will also be the primary representative of the Center to the outside world. We expect that the government, other universities, and industry will be very interested in learning from our experience at Illinois. The Director will have both the detailed knowledge and the broad overview necessary to convey that experience.

The *Policy Board* is the body which brings together the Center's users, the Scientific Director, and the professional staff to discuss policy issues. The Scientific Director will serve as the chairman of the Board. There are myriad detailed decisions on selecting or specifying equipment, setting priorities for its installation and support, software development timetable, establishing the desired job scheduling policy, etc. which require more formal consultation between users and staff. Without user influence in these issues, the research program of the Center could be compromised. However, users are not knowledgeable enough about the details of operations to do this by themselves. Therefore, the Board will meet every two weeks to insure a smooth and orderly growth of the facility, in a way that research throughput is maximized. The user members of the Board will be selected from among the primary users of the Center. These people will be rotated off the Board after two years, so that this duty does not seriously impact their scientific programs. This rotation will be staggered, in order to provide continuity.

The *Internal Allocation Board* will determine the amount of time that a University of Illinois researcher obtains. The Board will be composed of members of Illinois faculty chosen for their ability to judge the significance of proposed projects from a variety of fields. The review of allocations will be based on the research significance of the problem, the promise of the approach being proposed, and the record of the investigator making the proposal. In the case of extended large scale use, for which our Center will be almost unique, outside peer reviews will be requested. This allocation model has already been widely used on this campus for bulk computer funding and for internal funding of research proposals through the Graduate College Research Board (see Appendix C for details). Because of the original grant funding, the availability of funds from the researchers would not be a significant issue. The decisions of the Internal Allocation Board will be reviewed by the Program Committee periodically to ensure that high quality scientific research is being carried out.

Finally, we will establish a *Facilities Management Advisory Board* composed of the computer center directors of some of the leading research facilities in the United States. These people have an enormous combined expertise in setting up and running first class computational facilities. They will not only provide advice, but also assist in maintaining a cooperative interaction between our staff and theirs. We already have interest expressed for serving on our Board from:

Robert Ewald	- Director, Computing and Communications Division, Los Alamos National Laboratory
Hans Bruijnes	- Deputy Director, Computer Center, National Magnetic Fusion Energy Computer Center
Paul Rotar	- Manager of Systems Section of SCD, National Center for Atmospheric Research
Al Brenner	- Head, Computer Department, Fermilab
Saul Rosen	- Director, Computer Center Purdue University

We believe that this management structure will fulfill a number of goals. First, the facility will be largely directed by the scientific and engineering users and not by the computer staff. Second, access will be controlled solely by scientific merit. Third, a mix of internal and external users will be developed through collaborative research and the Visitors Program. Fourth, checks and balances will be instituted to guard against scientific provincialism. Fifth, an open flow of information about the system will be encouraged between users and staff. Finally, we will have a close coupling between our staff and the enormous repository of experience in the national laboratories.

There is well founded skepticism about the ability of a university to take on such a challenging task. While such a generalization may have a solid foundation, we expect the specific case of the University of Illinois to be evaluated carefully as part of a site visit. We point out, as a basis for claiming that we can successfully operate such a facility:

(1) We will build our system out of the functional subsystems developed at great expense at the national laboratories. This allows us to benefit from their present level of knowledge and achievement. Therefore we will not have to produce a new system, but can transfer a fairly mature approach to the campus.

(2) The campus is heavily committed to computing in research. In particular, the relationship between research groups and the computing center is remarkably collaborative rather than adversarial.

(3) Very large computing service projects have been taken on successfully, including the conversion of a large user population from a batch oriented IBM system to a timesharing Cyber system and the establishment of a statewide library support system.

(4) Building an integrated computational system out of functional subsystems is consistent with present plans, operations, and experience.

(5) Our Computing Services Office (CSO) has been successful at running identified facilities for the benefit of limited user groups, without mixing in the general campus computing load.

(6) The approach outlined later reduces the task to a series of well understood and achievable subtasks, rather than trying to create the whole system at one instant in time.

III.C. The Future of the Center

The development of the Center, and its associated computing resources, starts out in a very conservative way. It takes advantage of the opportunity to copy existing facilities, both to keep costs within reason and to make the undertaking feasible. The challenge in bringing such a facility into service is substantial and our plan is highly focused on this practical objective. A major step is the recruitment and training of staff. The size and composition of the staff is a balance between the need to activate the system rapidly, the benefits gained because many Center projects overlap activities already planned by CSO, and the realities of acquiring and absorbing a number of well qualified people in a short time. The time schedules and strategies for implementation recognize those factors. Within two to three years the Center should be through its initial problems and have a solid foundation for the future. Some aspects of that future require brief discussion here.

Since it is quite unlikely that there will be local computing facilities wherever supercomputers are needed, this center will address off-campus users from the outset. In the early years of the Center, we assume that visitors will spend some initial period at the Urbana site. Some remote access capability will support them after this period of familiarization, but the details of this will depend on the development of a national network and its funding. At a minimum, submission of batch jobs using one of the interactive front-end systems will be provided. For those who require the elaborate workstation support, remote access is unlikely to compete with a visit for effectiveness. As a national network comes into existence, and reaches the level of T1 transmission rates, workstation support will become more feasible. Output, in particular, can then be almost as good at a remote location as at a local one. Funding of this communication system and the workstations at remote locations is beyond the scope of the present proposal.

Being a national resource implies that a plan for continuity, at the state of the art, is a serious issue. Towards this objective we will take several steps: (1) We will attempt to establish a relationship with our vendor that keeps the computational and storage systems at the top of their product line; (2) we will seek to establish a permanent funding base for the portion of the system devoted to Illinois; (3) we will work with other sites to maintain consistency and standards so that remote users can have the flexibility to follow capacity; (4) we will gradually involve ourselves in developmental activities related to local research programs such as workstation development and evaluation, expert systems, software optimization, and networking of heterogeneous systems; and (5) we will be involved in the design and development of the national network.

The type of agreement we envision having with a vendor would also involve NSF. While we are presenting a specific five year purchase plan as our budget, we would like to build in the option for periodic upgrading of equipment in return for extending payments at a negotiated level. This could be in the form of an option, to be decided upon each time a major extension was necessary.

We expect that supercomputing, once introduced on the campus, will be important for the foreseeable future. Various sources of funds will be developed over the five years. Some basic support will be sought as part of the general operating budget, primarily from state appropriations. Other sources, such as new endowment funds will be sought, but more for use in programatic ways, such as research professorships or permanent facilities. Industrial contributions, as opposed to payments for services, are likely if industrial research programs benefit from contact with the Center.

IV. SCIENTIFIC AND ENGINEERING RESEARCH PROGRAM

The NSF's Press Report on Computational Physics (1981) makes a cogent statement explaining why supercomputers are *inherently needed* to simulate the complexities which arise in nature:

> "...In general, large-scale computation becomes necessary as the systems of interest become more complex. One moves from a few degrees of freedom to many degrees of freedom.
>
> Complexity emerges in different ways in the different subfields of physics. In some cases, it is in moving from ordinary differential equations to partial differential equations for the solution of interesting problems. This has happened, long since, in fluid dynamics and for the Schrodinger equation in non-central or many-body conditions, for radiative transfer problems in astrophysics, and in other areas. Alternatively, in such areas as nuclear reactions theory, many coupled integro-differential equations naturally arise and must be solved self-consistently.
>
> Complexity also increases dramatically when one moves from simple or one-dimensional models of physical processes, to realistic simulations. One sees this in research on the phases of fluids and solids and lattice models, in plasma simulations, in many-body calculations of galactic dynamics, and in quantum field theory.
>
> Complexity can come from the impetus to move from low order to high order expansions. This is the case in quantum electrodynamics and quantum chromodynamics; in high temperature and other expansions for liquids, solids, and lattice systems; and in high partial wave expansions for nuclear reactions. When the expansion techniques are algebraic, one moves from hand-algebra to algebraic symbol-manipulation on the computer.
>
> Complexity arises in moving from scalar systems to vector or tensor systems, and from linear systems to nonlinear systems. A striking example of this is General Relativity, whose partial differential equations are both tensor and highly non-linear. The fluid dynamics of many-component systems is another example.
>
> One sees, then, that complexity arises not from "bad taste in the choice of problems", but inevitably as theory advances. As one surveys the scope of subfields of physics...one finds over and over again that (i) there are important problems whose solutions must be found by computational techniques, and...(ii) that even the best investigators are resource-starved, with the facilities for accomplishing even the tasks already at hand."
>
> -Press Report, p. 6

This analysis can be applied to many other fields besides physics. It is this class of complex problems in science and engineering that our Center will focus on.

There will be two major groups of users of the Center: University of Illinois researchers and visitors from other institutions. Because we believe it is crucial to document the wide variety of important basic research in science and engineering that supercomputers can be applied to, we have done an extensive analysis of our University users. Presumably, an even richer array of research topics will be available in the visitor pool.

We have subdivided the University users into three subcategories:

(1) Large-scale supercomputer users.
(2) Potentially large users.
(3) New users from diverse disciplines.

Already active users would benefit immediately from the proposed supercomputer. This group (Table 2) represents 17 major research programs at the University of Illinois. These research programs involve about 25 professors at the University of Illinois, 92 graduate students, and 61 off-campus collaborators. For each of these primary users we have attached a brief proposal in Appendix A and have estimated their first year usage in Table 2. We urge the reader to spend some time reading Appendix A to see how essential the supercomputer has become to so many frontier fields of basic research.

In the Natural Sciences, studies in astrophysics, quantum field theory, material properties, quantum chemistry, and atmospheric sciences are represented. In Computer Science a wide range of studies in supercomputer architecture, software, and algorithm research will be carried out. In the Engineering Sciences, fundamental problems in electrical, chemical, nuclear, and mechanical engineering are being addressed. Most of these researchers are world leaders in their fields.

A number of this first group are already using 100 hours of remote supercomputer time or 500 hours of local general purpose machine time per year. That rate of usage is set by availability of processor power. With the high speed integrated facility we propose, some research groups of 8-12 investigators, such as those listed in Table 2, have computing requirements up to 1000 CRAY-1 equivalent hours per year. Thus, this first group has easily recognized demands and the ability to translate these demands into actual utilization. Much of the large-scale computing presently done by this group occurs away from the campus (for location see Table 2 and Appendix A). The largest campus facility is a Cyber 175, which is not fast enough (approximately 0.1 CRAY-1) and has insufficient central memory (262K words) to accommodate the largest-scale users (for detailed comparison, see Sec. V.B.1). The proposed Center will allow this group to carry out innovative large-scale computing in an interactive and stimulating local environment that should increase their knowledge and productivity enormously.

The second group of users includes approximately 50 additional faculty members along with their collaborators and graduate students. This group represents a more diverse set of research areas, but their progress has been more limited because of lack of access to large scale computer facilities. They would create some initial load on the system and some would become part of the next generation of large users. Brief descriptions of their research interests are included in Appendix B and their topics are listed in Table 3. Anyone who has dealt with large-scale computing over a period of time is aware that once the computer is available to attack a problem, not all of these problems will prove to be manageable or interesting. We are under no illusion that each person who can think of a problem that requires a supercomputer, would either undertake that problem or become a regular large-scale user. Given the availability of such a system, however, many of these users can be expected to become active in the use of supercomputers and will take a greater part in the Center's activities.

TABLE 2

Summary of Group I Users

RESEARCH AREA OF PROPOSED SUPERCOMPUTER USE	CURRENT COMPUTER USAGE (HRS/YEAR)	PROJECTED FIRST YEAR USAGE (CRAY 1 EQUIVALENT HOURS)	CURRENT NUMBER OF GRADUATE STUDENTS/ COLLABORATORS AT OTHER INSTITUTIONS	FACULTY AT U OF I	POSITIONS
Relativistic Astrophysics	100 Cyber 175 200 CRAY-1A (MPI, LLNL)	1000	3/5	Smarr	Assoc. Prof of Astronomy and Physics
Stellar Evolution	500 Cyber 174/175	600	3/6	Iben	Prof. of Astronomy
Star Formation In Magnetic Interstellar Clouds	150 Cyber 175 20 CRAY-1A (MPI)	800	2/3	Mouschovias	Prof. of Physics & Astronomy
Gauge Theory And Elementary Particle Physics	50 CRAY-1A (LANL) 300 CDC 7600 (LANL) 500 Cyber 175 200 FPS-164	1000	5/7	Kogut Wyld Stack Stone	Prof. of Physics Prof. of Physics Prof. of Physics Asst. Prof. of Physics
Electronic Structure of Solids	500 FPS-164	100	4/5	Kunz	Prof. of Physics
Disordered Solids	1000 Urbana Monte Carlo Machine	100	1/2	McMillan	Prof. of Physics
Many Body Systems	200 Cyber 205 (Bochum) 200 IBM 370/195 (Argonne)	400	2/3	Pandharipande	Prof. of Physics
Large Molecule Electronic Structure	500 Cyber 175 5000 VAX 11/780	100	4/3	Dykstra	Assoc. Prof. of Chemistry
Chemical Quantum Dynamics in Condensed Phases	2000 VAX 11/780	300	5/4	Wolynes	Prof. of Chemistry
Global Atmospheric Simulations	20 CRAY-1A (NCAR)	100	2/1	Ogura Soong	Prof. of Meteorology Assoc. Prof. of Meteorology
Dynamics of Sea Ice	30 CRAY-1A (NCAR)	100	1/2	Walsh	Assoc. Prof. of Meteorology
Dynamics of Convection	150 CRAY-1A (NCAR) 200 VAX 11/780	1000	3/5	Wilhelmson	Prof. of Meteorology
Supercomputer Architecture, Software and Algorithm Research	1200 IBM 4341	200	20/6	Kuck Sameh Lawrie Gajski	Prof. of Computer Science Prof. of Computer Science Assoc. Prof. of Computer Science Assoc. Prof. of Computer Science
Semiconductor Multidimensional Device Models	4000 Harris 800	200	12/1	Hess Holonyak	Prof. of Electrical Engineering Prof. of Electrical Engineering
Physics of Turbulence	35 Cyber 175	100	15/3	Hanratty	Prof. of Chemical Engineering
Flow and Fracture of Structural Materials	50 Cyber 175 50 IBM 4341	100	3/4	McMeeking	Assoc. Prof. of Theoretical and Applied Mechanics
Fusion Plasma Engineering	90 Cray-1, 1S (NMFECC) 110 CDC 7600 (NMFECC)	300	8/1	Miley	Prof. of Nuclear Engineering

This table summarizes the proposed use of the supercomputer by the first group of users. Members of this group intend to make immediate use of the facility. The 25 faculty members are the lead individuals involved in the research areas listed. They represent a large number of other faculty, post docs, students and off-campus collaborators. A breakdown of the current number of students (92) and the number of collaborators from other universities, industry and national laboratories (61) is indicated. Current computer use for each research area is included in terms of hours per year. The machines used are at the University of Illinois unless otherwise indicated. The projected computer time is estimated in terms of CRAY-1 equivalent hours. We estimate that a CRAY X-MP will deliver at least 12,000 CRAY-1 equivalent hours in a year. The Group I users will require about 1/2 of this time. Appendix A contains further information on the research to be carried out.

TABLE 3

Summary of Group II Users

Department	Research Area	Researchers	Position
Physics	Experimental Particle Physics	Brown and 9 other faculty	Professor
	Light-Energy Transduction in Biomolecules	Eisenstein	Assoc. Professor
	Physics of Biomolecules	Frauenfelder	Professor
	Accretion by Compact Objects and Stellar Dynamics	Lamb	Professor
	Nuclear Structure and Scattering	Ravenhall	Professor
Astronomy	Data Processing of VLA Observations	Dickel	Res. Assoc. Professor
	Radiation Hydrodynamics of Molecular Cocoons	Dickel	Res. Assoc. Professor
	Chemical Astrophysics	Snyder	Professor
	Hydrodynamics of Nova Explosions	Truran	Professor
	Explosive Nucleosynthesis	Truran	Professor
Chemistry	Intramolecular Dynamics of Molecules	McDonald	Professor
	Molecular Scattering Theory	Secrest	Professor
Computer Science	Numerical Methods	Gear	Professor
	VLSI Design Automation	Kubitz	Assoc. Professor
	VLSI Design Automation	Gajski	Assoc. Professor
	Iterative Solution of Large Systems of Linear Algebraic Equations	Saylor	Assoc. Professor
	Supercomputer Design and Application	Slotnick	Professor
	Simulation of Semiconductor Devices	Watanabe	Assoc. Professor
Atmospheric Sciences	Dynamics of Liquid Drops	Beard	Assoc. Professor
	Climate Modeling	Trenberth	Professor
Chemical Engineering	Chemical Process Design	Stadtherr	Assoc. Professor
Electrical Engineering	Circuit Simulation and Design Evaluation	Davidson	Professor
	Circuit Simulation and Design Evaluation	Abraham	Assoc. Professor
	Inverse Problems in High Resolution Image Reconstruction	Jenkins	Assoc. Professor
	Evaluation and Design of Communication Systems	Pursley	Professor

Department	Research Area	Researchers	Position
Mechanical and Industrial Engineering	General Radiation Transport Calculations	Buckius	Assoc. Professor
	Modeling of Gas Dynamics	Chow	Professor
	Hydrodynamic Shock Physics	Krier	Professor
	3-D Flow Fields in Combustion Chambers	Peters	Professor
Theoretical & Applied Mechanics	Comparison of Simulated Turbulence with Experiment	Adrian	Professor
	System Identification and Reliability	Bergman	Assist. Professor
Civil Engineering	Structural Optimization	Haber	Professor
	Structural Mechanics and CAD/CAM	Lopez	Professor
	Groundwater Contamination	Valocchi	Assist. Professor
Aeronautical and Astronautical Engineering	Computational Gas and Fluid Dynamics	Yen	Professor
Anatomical Sciences	Biomechanics of Cell Sheets	Mittenthal	Assist. Professor
Genetics and Development	Simulation of Living Cells	Futrelle	Research Scientist
Physiology and Biophysics	Emergent Oscillatory Properties of Neural Networks	Jakobsson	Assoc. Professor
Accountancy	Multiple Time Series Analysis	McKeown	Professor

The third group of users will come from those who join the University because of the availability of our facility or those who, once familiar with the environment, begin to select research problems that require supercomputing. National laboratories are mission oriented (e.g. nuclear weapons, aerodynamic design, magnetic fusion, atmospheric sciences, etc.). They have been unable to provide much opportunity for investigators outside of these areas to consider the supercomputer as a potential instrument for their research. Thus, the machines are used only within a very few selected disciplines and their applicability to other areas is largely speculative. The supercomputer systems at universities and service bureaus serve a wider clientele, but the financial barrier has limited their impact. We consider the addition of a fully equipped supercomputer, with no financial hindrance, a critical step in addressing this problem. We envisage that innovative research will be done in diverse areas by this third group.

The second major pool of users are those choosen by the Program Committee in a national solicitation. The visitors will enhance the Center by sharing their expertise with the University of Illinois community of users, while gaining access to substantial amounts of computer time. For the reasons outlined in section III.A., we believe that it is essential that the supercomputer facility be located in a strong research-oriented university. However, it is important to note that the number of off-campus collaborators and visitors to our Center will equal or exceed the number of on-campus faculty users. Thus, it is clear that our proposed Center will have a decided national impact.

V. THE SUPERCOMPUTER SYSTEM CONFIGURATION

V.A. Principles of a Well-Balanced System

A supercomputer must be an integral part of a *well-balanced computational system* to be used to its full potential for basic research and design engineering. Our experience in using various of the world's existing supercomputer systems (e.g. LANL, NMFECC, LLNL, NCAR, MPI) has taught us that there are several crucial *functional subsystems* other than the supercomputer itself in a first-rate configuration (see Figure 1). There must be a subsystem for very high speed communications to handle the enormous information flow to and from all the other subsystems. Users are most effectively served on powerful local nodes for pre- and post-processings and display of data. A large capacity online storage facility for user files, which is instantly accessible, is needed to hold the enormous amount of output data submitted to and produced by the supercomputer. Finally, a high volume centralized output facility is needed which can quickly produce paper, film, and video hard copy of high quality.

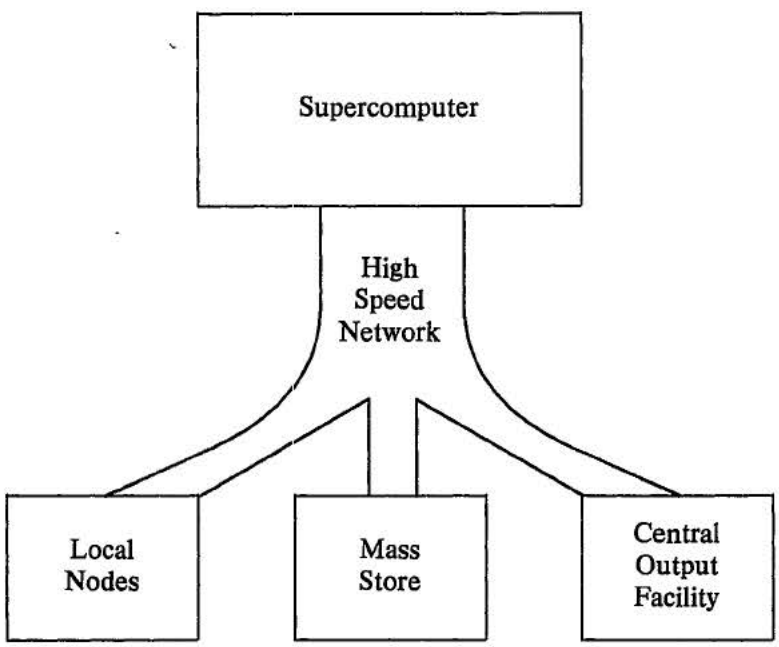


Figure 1: The Integrated System

The heart of the proposed system is the fastest, largest in memory, most reliable, and easiest to use machine which is currently available. It has multiprocessor architecture, not only for higher throughput, but also because *multiprocessing represents the future direction for growth in supercomputers.* Users must begin to learn to write codes on multiprocessors, just as they have already had to learn to use pipelined (vectorized) architecture on previous supercomputers.

The enormous throughput of such supercomputers can only be realized if there are *no bottlenecks* in the rest of the system. One must view a supercomputer system as a high speed network for information flow. The productive output is limited by where the flow is most constricted. It makes no economic sense to pay the capital costs of a supercomputer, unless one also pays the requisite costs to avoid such constrictions. We believe that the proposed system is the minimum configuration which will allow full utilization of the supercomputer power.

The system configuration, as already mentioned, consists of *functional subsystems* (see Figure 1). The underlying idea is to have modules that specialize in performing certain functions very well and that can

still be used when another module is added or replaced. Also, functional subsystems can be upgraded individually as the need arises, without bringing the entire system down. Without modularization, an integrated reliable supercomputer system of the complexity that we propose would be almost impossible to create.

The key to integrating the functional subsystems is a *high speed communication network.* This is the major factor in our view that makes the Livermore and Los Alamos systems so powerful. Users can interactively use the supercomputer just as they would their own personal work station or mini-computer. Further, there is enormous economy-of-scale in centralizing all file storage and major output devices. With a high speed network, access times to huge files are measured in seconds. Powerful local nodes, with their own processors, can do many routine duties (text editing, graphics, code development), so that more supercomputer time is available for scientific and engineering research. But the major effect is that the network turns the supercomputer into a true research tool. It is available to help the researcher at every instant. It works on his time scale and with his research schedule. Our experience is that when one goes from a supercomputer site with a high speed network to one that does not have such a network, then the scientists time becomes dominated by nonscientific issues such as data transport.

Once the functional subsystems are networked, *powerful systems software* can aid in enhancing research productivity. Time-sharing operating systems are well developed at several national laboratories (LANL, NMFECC, LLNL) for working on supercomputers across a high speed network. These systems not only allow one to work interactively on the supercomputer, but they also contain sophisticated standardized utilities such as debugging, editing, graphics, file manipulation, etc. This "toolbox" of utilities is essential for code development and post-processing of runs that require the supercomputer. On local nodes we expect that UNIX will be used extensively as the operating systems for minicomputers, work stations and personal computers. This popular operating system is becoming the defacto standard. At both the supercomputer and the local node levels of our system, the *standardization of systems software* will be crucial to allow users to work on any device in the network.

The *automation of output* is another important part of our system. It is unacceptable for a talented researcher to run a problem in ten minutes on the supercomputer and then spend a day waiting for a graph or movie showing some result of the calculation. With the combination of powerful local nodes and a high speed network, most forms of medium resolution output (numbers, line graphs, colored images, movies, etc.) will be quickly available electronically on the monitor of the local user. Local nodes will have some low volume hard copy devices (printers, plotters, Polaroids, video tape, etc.) for "quick-look" uses. A centralized output facility will have high volume paper, film, and video devices to produce publishable quality hard copy with fast turnaround for even large quantities of output. After the initial period of installation and breaking in, we will devote considerable staff support to providing standardized graphics software for the wide variety of researchers that our Center will accommodate.

The *high priority on high-resolution graphics and color images* is a central feature of our proposed system. As extremely high resolution computations become possible, because of the high speed and large memory of the supercomputer, the numerical output becomes unmanageable unless it is presented in graphical form. Our major users in natural sciences (e.g. hydrodynamics, atmospheric sciences, molecular structure), in computer science (e.g. VLSI design), and in engineering (e.g. computer aided design, structural mechanics) are dependent on imaging to understand the results of their numerical simulations. Furthermore, these images can be the primary stored form of the results of the calculation. Their storage and transmission through the network represent some of the major demands on engineering of the system's information flow capacity. Also the images must be in device independent metacode, so that they can be easily accessed by different graphics terminals or hard copy devices anywhere on the network.

If the users, particularly visitors, are to fully utilize our system, there must be an *open flow of information* between all people on the system. This includes user to user, user to staff, and staff to staff. The flow must be two way with users being constantly updated on system changes, and users having access to consulting staff to answer their questions or complaints. Artificial barriers between staff and users will be discouraged. The users will be encouraged to learn any aspects of the operations that could improve their productivity. Researchers often choose computing hours at night or on weekends to get faster throughput. This should be encouraged to reduce peak loading of the system. However, this means operational support must be available 24 hours a day, 7 days a week.

In creating an integrated system we plan to *build on existing strength* whenever possible. Locally we have a large Computing Services Office (CSO) which has experience in managing a campuswide computer system as well as aiding in the development of more specialized facilities around the campus (see Appendix C). The proposed system is being designed as much as possible to utilize an operating system, high speed network, mass storage subsystem and output subsystem already proven in the national labs. Our integration of minicomputers, work stations, and personal computers into the high speed network and operating system will borrow heavily from similar efforts at LANL, NMFECC, and LLNL. Whenever possible we will use emerging standards system wide. Therefore our major initial effort will be the smooth connecting of subsystems into an integrated system.

Realistically, the fully configured system will take some time to establish. However, we feel that it is essential to have a productive working system as soon as possible. Accordingly, we have devised a *buildup strategy* to phase in the system. This strategy will be made explicit in the next section.

V.B. Selection of a Supercomputer

V.B.1 Why a Supercomputer?

It is often said that rather than buy a supercomputer to serve many users, it makes more sense to buy slower speed computers (array processors, superminicomputers, etc.) and dedicate them to small research groups. This has, in fact, been done by a number of primary user groups (Table 2) in this proposal. Although we find such machines to be indispensable at our local nodes for code development, graphics, post-processing of supercomputer runs, editing, etc., they are in no way a substitute for a supercomputer. The best test of that statement is that many of these primary users still fly to or remotely use supercomputers for their work.

The major advantage of the supercomputer speed is that it allows one to make scientific progress on a human time scale. Code development requires many hundreds of trial runs. If these take a few minutes on a supercomputer one can get through many trial runs per day and be ready for a much improved several hour production run overnight. On a fast array processor, a ten minute supercomputer job takes over an hour, and on a superminicomputer nearly twenty-four hours. Thus, what should be simple code checks can only be run overnight. This can reduce scientific productivity enormously.

The power and uniqueness of a supercomputer can be characterized by comparing execution times of the same code on a supercomputer to machines traditionally available to University scientists. For explicitness, we use the CRAY 1-A for comparison. For number-intensive calculations for which vectorized codes can be written, one can achieve a good fraction of the CRAY's optimal speed of 160 million floating point operations per second (MFLOPS), using FORTRAN programming, *if* several simple rules are followed in the construction of the program's repetitive DO loops. Utilities available on the operating system CTSS, used by LANL, NMFECC, and LLNL, allow the user to identify those loops which the CRAY compiler runs in a vector mode and to optimize the codes easily. An even more powerful tool (Paraphrase), available at the Laboratory for Advanced Supercomputers at Illinois, can restructure codes to make very efficient use of machine architecture. In addition, math libraries such as SCILIB and CALMATH, supported at LANL, contain optimized subroutines written in CRAY Assembly Language (CAL) which provide vector speeds to the user without the need of the scientist to delve into architecture considerations. Of course, many scientific calculations are not fully vectorizable (IF statements and extensive I/O both inhibit vectorization), but substantial gains in execution speeds can be achieved, nonetheless, if the calculation-intensive parts of the code are vectorized effectively. Simulations in gauge theories, hydrodynamic calculations, etc. are accelerated enormously by intelligent programming.

Consider an interesting, realistic example. Computer simulations of Quantum Chromodynamics depend upon fast Monte Carlo algorithms for SU(3) gauge fields. A vectorized version of this code was found to run 10 times faster on a CRAY 1-A than on a CDC 7600. However, if the same problem were programmed without vectorization, then the CRAY 1-A exceeded the speed of the CDC 7600 only by a factor of 2.5. Comparative testing against a mid-sized array processor, the FPS-164, yielded comparable results -- for a vectorized SU(3) program the FPS-164 achieved speeds of 1.0-1.5 CDC 7600's which left it 6-10

times slower than a CRAY 1-A.

A very simple benchmark study was recently made to illustrate these points. A program which simply multiplied two 3 x 3 matrices one million times was written in a vector fashion for a CRAY 1-A and a FPS-164 for comparison with scalar, optimized FORTRAN codes run on a Cyber 175 and a VAX 11/750 (with floating point accelerator). The CRAY-1A ran at 70 MFLOPS, the FPS-164 at 6 MFLOPS, the Cyber 175 at 2 MFLOP and the VAX 11/750 at 0.2 MFLOP.

As one last example, a two-dimensional general relativistic hydrodynamics code was developed on a University of Illinois VAX 11/780. On the scalar Cyber 175 it ran 10 times faster and, with a few days of vectorizing the code, it ran 200 times faster than the VAX on the CRAY 1-A at Max Planck Institute. Eight-hour overnight runs on the VAX could only be made on a very coarse spatial grid (20 x 30 zones). On the CRAY these same runs took 2 minutes, so many of them could be run during the day. Overnight on the CRAY, one could run one hour jobs on a more finely zoned (50 x 100 zones) problem. Finally, each weekend one could run high resolution (100 x 200 zones) production runs which last ten hours. Thus, in one week at a supercomputer center such as we propose, one researcher can get 15-20 hours of CRAY time, equivalent to a years access time (4000 hours) on a dedicated VAX level machine.

The lesson here is simply that a supercomputer is 1) capable of speeds one to two orders of magnitude greater than those presently available on other systems, and 2) that it must be programmed properly to achieve a good fraction of its capability. The prospect of developing parallel processing on multiple central processing units (CPU's), as in a CRAY X-MP, should lead to even greater gains in speeds and should yield insights for additional growth of computer architectures for scientific applications.

V.B.2 Our Objectives

To help guide our choice of the supercomputer we have set up goals for the Center during the next 5-10 years. We can break down the development of the system into three parts:

Near Term: To provide supercomputing power to our scientific and engineering community as quickly as possible.

Intermediate Term: To provide one of the world's fastest and easiest to use, integrated supercomputer facilities.

Long Term: To provide a very competitive facility that can grow and adapt to our user's expanding requirements into the 1990's.

To achieve our *Near Term Objective* we must consider systems that are currently available, i. e. for sale at the time we are funded. While there are always promises of new and better systems on the horizon, the urgency of our needs are such that it seems counterproductive to consider such promises if they are not backed by benchmarkable systems. The only two supercomputers available for sale today in the American market that may potentially satisfy our objectives are the CDC Cyber 205 and the CRAY X-MP. The recently revealed Cyber 2XX is not currently scheduled for delivery until 1987 and the CRAY 2 has undergone several schedule slips. Preliminary discussions with both CRAY and CDC have indicated that their basic system configurations could be installed within a year of funding.

Both the 205 and the X-MP allow pipelining (vectorization) to speed up scalar codes. However, the majority of our supercomputing faculty have used CRAY-1 systems, since Cyber 205 systems have not been available to them through networks or national labs. It is very important to have available the developed and proven CRAY-1 software base, all of which is compatible with the CRAY X-MP. We have reviewed the activities at several national laboratories that have CRAYs (NCAR, LANL, NMFECC, LLNL). These have highly sophisticated and proven sources of utilities, graphics, and other software which would be readily transferable to a CRAY at Illinois. Some of the labs have already indicated a willingness to support cooperative activities, including temporary loans of personnel, sabbatical leave for their staff to visit here, and free exchange of much software and information.

Most of the major Departments of the University of Illinois which have an interest in large scale

computing currently possess local superminicomputers (VAX 11/780 level) with their own disks and hard copy units. We will hook the supercomputer to the high speed network that Illinois is currently installing and use the existing Departmental facilities as local entry nodes. This network is built around the Network System Corporation Hyperchannel.

The CRAY X-MP can be operated under the Cray Time Sharing System (CTSS), used at the national labs (LANL, LLNL, NMFECC, SANDIA,...). This is a proven, reliable, sophisticated, and very powerful operating system. It works in a Hyperchannel network environment (LLNL), and the labs support most of the potential local nodes we want to use (VAX, SUN, IBM PC, etc.). Informal discussion with the labs indicate that we could quickly bring up the system on our network and that they would help in the training and maintenance required. In particular, Los Alamos will be about one year ahead of Illinois in bringing the CRAY X-MP up under CTSS, including integrating its Input/Output Subsystem (IOS), Solid State Disk (SSD), and multiprocessors.

We will be able to set up a mass storage and centralized output facility very quickly by copying the highly successful Common File System (CFS) and Print and Graphics Express Station (PAGES) of Los Alamos National Laboratory. These facilities, described in detail below, can handle the high volume produced by a supercomputer. The development of the software and hardware configuration in these two subsystems has required some 50 man-years at LANL. We will purchase the minimum hardware necessary in the first year, and get the LANL software running on it. This will allow large-scale research problems to be documented and archived very soon after the supercomputer begins operation.

Assuming funding approval in April 1984 the central system components would be delivered over the next twelve months, with the processor installation likely about January 1985. Because of the close association between this project, other CSO plans and the collection of equipment presently available, a great deal of the integration work could take place while waiting for the processor. In short, by the end of Fiscal Year 1985, we can get all of the major subsystems in Figure 1 up, so that users will be able to take full advantage of the processor speed as soon as possible. Staff recruiting can begin immediately in the knowledge that there will be useful work to do prior to installation of the complete system.

In the following few years of funding, our *Intermediate Objective* is to expand our system into one of the highest throughput, easiest to use, integrated supercomputer systems in the world. Here we will build on the high-speed Hyperchannel network and the CTSS operating system (by then already installed).

The desire to have a supercomputer with multiprocessor capability is very strong at Illinois. Multiprocessor means having two or more complete central processing units (CPU's) inside the same machine (see Figure 2). Initially such a machine would be used essentially as two separate processors. This will allow us to run large scale production jobs around-the-clock on one processor, while at the same time many smaller jobs are being time-shared on the other processor. This is crucial to our goal of using the supercomputer to solve major breakthrough problems which require very long runs (approximately 100 hours) while simultaneously meeting the needs of other users. The CRAY X-MP satisfies this goal perfectly. The throughput increase over the CRAY 1-S is about two to three, with half of that factor coming from each processor.

One of our goals at the Center is to be able to attack problems which are currently memory limited (e.g. 3-dimensional hydrodynamics or lattice gauge theory). For these types of problems, the amount of fast memory needed exceeds the 1-4 million words available on, say, the CRAY 1-S, and so the time to execute the problem is prohibitive because it must be swapped in and out (approximately 4 million bytes per seond) of memory onto temporary storage rotating disks. The memory hierarchy (Figure 2) of the CRAY X-MP solves this problem for us. It has a large (4 million word) internal memory which is coupled to a very large (32 million word) external fast memory (SSD) through an enormously high speed (approximately 1000 million bytes per second) channel. This will allow an order-of-magnitude increase in the size of a problem which can be handled at supercomputer speed. Furthermore, we may be able to greatly speed up the response of the system to timesharing by leaving frequently called files (compilers, editors, etc.) on the SSD, rather than swapping them in and out of disk all the time. Clearly the SSD is not a substitute for the very much larger capacity (greater than 1000 million words) temporary storage disks, but it will allow our system to handle calculations never before attempted.

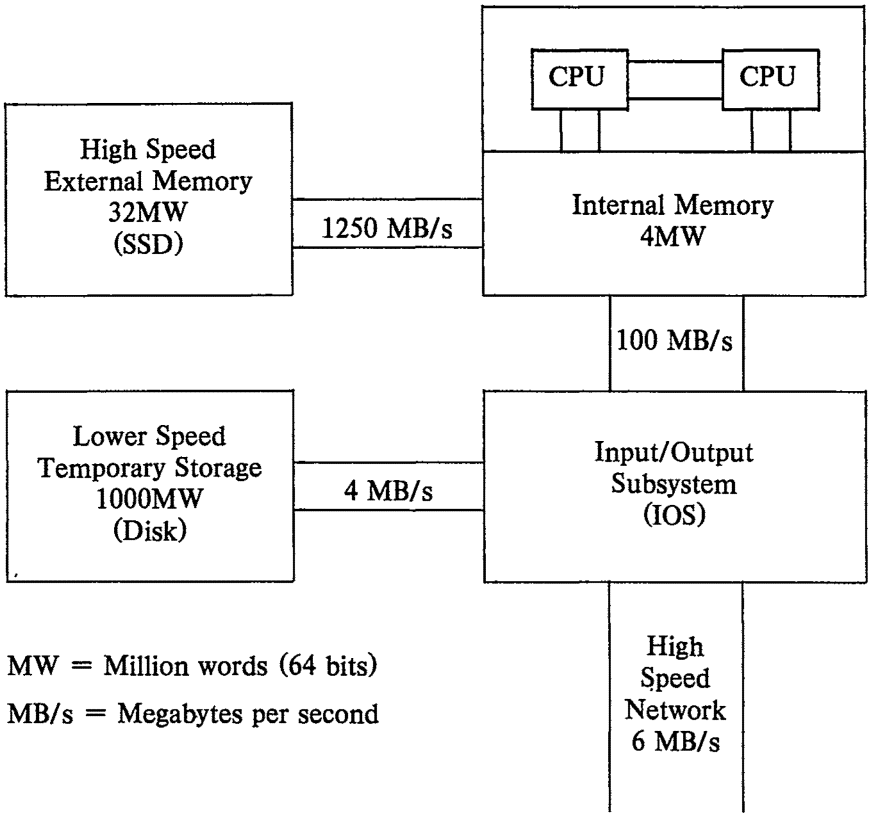


Figure 2: The Supercomputer

As our user load increases, we expect to add capacity to our mass storage and centralized output devices. In addition, we expect to begin moving users onto powerful scientific work stations (e.g SUN or APOLLO) or IBM personal computers clustered in academic departments on Ethernet-like (approximately 1 million bytes/sec) nets in their respective buildings. The separate buildings would be linked via gateways onto the broadband campus cable. There are already major programs to bring up smart terminals in the CTSS environment at LANL, LLNL, and NMFECC. We will again profit enormously by using the techniques developed by the national laboratories.

Besides hardware development, the Center will foster a close relationship between the users and the Laboratory for Advanced Supercomputers at Illinois. The LAS Parafrase system can, in many cases, automatically restructure user programs so that they can take advantage of the vector speed, multiprocessor architecture, and the memory hierarchy of the supercomputer.

The *Long Term growth objective* for the next years is the most difficult to assess. The architecture of the X-MP appears to allow expansion in several ways, and we believe that Cray Research will be considering such expansion. Both the main memory and SSD sizes could be greatly increased and they could be operated at higher bandwidths (via more bank parallelism). Furthermore, additional processors could be added. Even the present processor communication hardware should support four processors, two more than initially advertised. Thus, more throughput and/or better turnaround should be possible in a few years. This potential growth with the same base system and common software is another argument for the CRAY X-MP at this time. Similar enhancement of the Cyber line in the recently revealed Cyber 2XX will be evaluated nearer the time of the decision.

V.B.3 Summary

In section V.B.2 the CRAY X-MP is identified as the probable system of choice. While we do expect to make a careful evaluation of it in comparison with other systems, there are several justifications that led us to work with it. Budget requirements for alternative systems are sufficiently close that it is representative of this class of machines. The justifications are as follows:

(1) Present use by University of Illinois scientists is mainly on CRAY-1 systems.

(2) The CRAY system is more mature in a software sense, with compatibility between the various models, including the CRAY X-MP.

(3) Proven sophisticated and integrated operating systems, mass storage devices, and centralized output facilities will be available from the national laboratories for use on the CRAY X-MP.

(4) The multiprocessor architecture and the sophisticated memory hierarchy of the CRAY X-MP will allow new types of research problems to be attacked.

(5) Existing benchmark data indicates the competing choices are roughly comparable in compiled program speed.

(6) The system is already in use in a Hyperchannel configuration, whereas the CDC Loosely Coupled Network (LCN) is not a generally attractive alternative at this time.

(7) The growth path is fairly clear, conservative, and builds on existing strengths.

Of course, our minds are open and during the review period for this proposal, we will be carefully considering our specific configuration choices and the calendar for system growth. This effort, together with new equipment announcements could modify our plans. While the remainder of this section uses the CRAY X-MP for discussion purposes, a different choice of equipment would not materially change most aspects of the configuration and hence the costs would not vary sharply from those in the proposed budget.

V.C. Distributed Network

V.C.1 The High Speed Network

Our proposal is to create an integrated supercomputer system, built from multiple subsystems. Interconnection of the major subsystems is through the use of the Network Systems Corporation Hyperchannel. Complementing this, for specialized point-to-point connections, is the campus broadband coaxial cable system which reaches most campus buildings. (An example of this need would be interconnection, via gateways, of several local area nets serving buildings.) This cable supports both high speed modem pairs and lower speed networking products such as Sytek and Ungermann-Bass, as well as video. When the requirements anticipated do materialize, it will also be necessary to add fiber optic links for very high-speed paths and to use the video capabilities of the broadband system. With the exception of fiber these are all areas of technology with which the campus has extensive experience.

The Network Systems Corporation's Hyperchannel was originally chosen for the network because it supports the majority of the systems of interest to the campus. It is already in use at several CRAY installations and provides the capacity necessary. The campus is already beginning to use Hyperchannel as the means of interconnecting its major computing systems, and we plan on it as the means of integrating the subsystem architecture. A campus map (Figure 3) shows the location of major equipment. High speed local networks will be necessary in buildings with large concentrations of workstations, and gateways to the broadband cable will be necessary. The engineering of this network of data transmission facilities will be responsive to the needs of users at their most logical working location.

The access to the supercomputer will be developed in two phases. In the first phase the dedicated computer in user departments will be connected via a Hyperchannel, either directly or via a broadband link, to provide high-speed (6 million bytes per second) file transfer. Postprocessing of supercomputer runs on the dedicated computers will be achieved very early in this way, and will be available as soon as the initial system is operational. These systems will remain an important means of access because of user familiarity and because of the special devices that are attached. This will be enhanced by terminal or personal computer access located in the office or laboratory areas of the investigators. The second phase will upgrade the local nodes. This is described in section V.C.4 and 5. The Hyperchannel will also be used as the means to provide network wide services to all major machines, including the CRAY X-MP. Examples of such services are discussed below (V.C.5 and 6) and include archival storage, microform production, and bulk printing.

This proposal includes expansions of the Hyperchannel to interconnect the Computing Services Office facilities in the Digital Computer Laboratory, the peripherals and CRAY processor which are to be located in the Astronomy Building, and several departmental machines (including one or two FPS-164 systems), in at least four other buildings where major use will originate.

V.C.2 The Supercomputer

The supercomputer will be located on the second floor of the Astronomy building. Although the Astronomy building was constructed for the purpose of housing ILLIAC IV, the machine never came on campus and some of the associated air conditioning and power requirements were never completed. The machine room and its support systems need major renovation for this, as well as a small amount of renovation to house the proposed staff. The equipment shown in Figure 2 will reside there as well as the key staff support. Pending a detailed site analysis, we do not know whether the mass store and centralized output facilities (see below) will be housed at the same site or connected via Hyperchannel to the Digital Computer Laboratory (DCL, Figure 3). In any case, human intensive activities, such as tape mounting, will probably be in DCL.

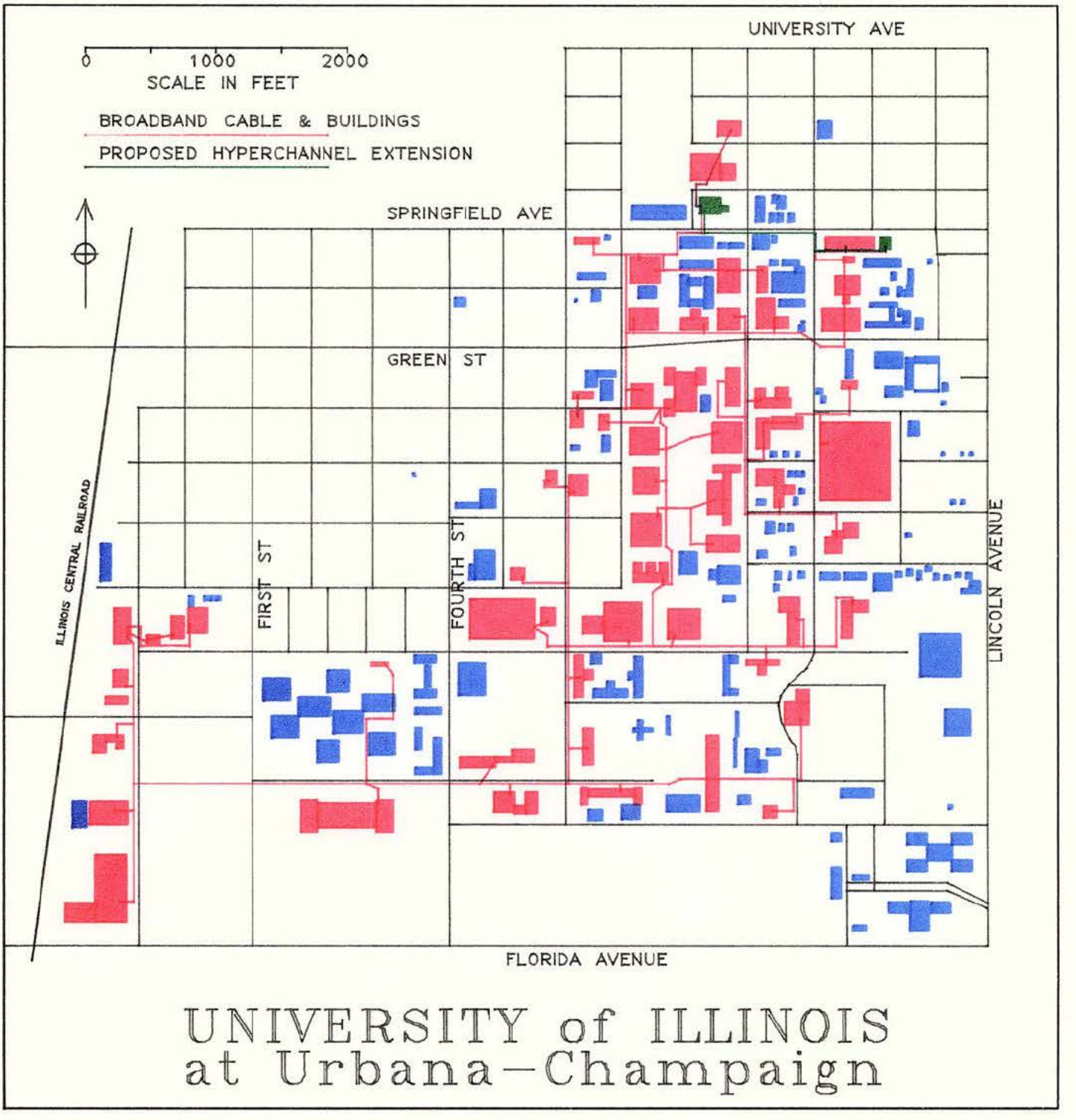

UNIVERSITY AVE
0
1000
2000
SCALE IN FEET
BROADBAND CABLE & BUILDINGS
PROPOSED HYPERCHANNEL EXTENSION
SPRINGFIELD AVE
GREEN ST
ILLINOIS CENTRAL RAILROAD
FIRST ST
FOURTH ST
LINCOLN AVENUE
FLORIDA AVENUE
UNIVERSITY of ILLINOIS
at Urbana-Champaign

Figure 3

V.C. 3 Local Nodes

The Press Report recognized the crucial need for considerable processor power at each local node:

> "To the scientific user, the local nodes make possible modes of operation and scientific investigations not possible via remote access to a central node. Since a typical local node is shared among a much smaller number of users than a central node, there is much greater ability to adapt computer operations to the requirements of the user. The machine may be dedicated or adapted to a special project for some period of time with much less disruption than would be the case with supercomputers at the central node. Further, the allocation of resources at the local node can be much more flexible than at the central node; some of the computation time can be allocated without formal and lengthy justification.
> -- Press Report, p.27

Thus, we expect local nodes to have the same diversity as the research groups' areas of interest. However, to maintain transparency of the network we cannot support every possible piece of equipment on the node. To try to encourage flexibility while maintaining system consistency, we will use a two-pronged approach.

First, we will establish a Model Local Node at the site of most of the Center's activities. It will be fully equipped with most of the devices users would want at their local nodes. The Center's staff will develop uniform software for integrating the devices into the system. All users will be encouraged to try out the devices and interact with the staff in the development process. Then as need arises at other local nodes, some funds will be made available for replicating the device and its software at that local node. Thus, we avoid over-equipping the local nodes while providing access to specialized equipment for all users at the Model Local Node.

Second, we will attempt to implement emerging *de facto* standards in hardware and software. Detailed study will be made before the funds are spent, but some probable examples are: (1) Hyperchannel for high speed networking, branching to lower speed Ethernet on local smart terminal clusters (see Figure 4); (2) Intel Multibus or DEC Q-bus for local processors; (3) UNIX as the operating system on local processors, etc.

The basic structure and use of our local node (Figure 4) is just that foreseen in the Press Report:

> "As the capacity of the Computational Physics System increases, it will be essential to increase both the capacity and the capabilities of graphics devices at the local nodes, in order to manage the ever rising data flow. An efficient method is to establish a Data Management Facility (DMF) capacity. A typical DMF would consist of four subsystems: Controller, Display, Storage, and Hard Copy. The Controller is a small computer which acts as a data receiver from the other nodes or local computer and as a switchyard within the DMF. The Display subsystem contains as many graphics display devices as required by the research group. The Storage subsystem consists of disks or tapes on which images or numerical data are stored. Hard Copy devices include line printers, plotters, or screen copying devices.
>
> "Such a loosely coupled system can be upgraded as demand requires. Adding capability can be achieved by updating only one subsystem at a time. We stress that one critical feature of the system is data rate to the screens in the DMF. these must be high enough that a picture appears instantly upon request. This is because managing data graphically may require the scanning of hundreds of images per session at the console.
>
> "A scientist would typically use the DMF for post-processing of calculations run at

either the local node or the principal node. The numerical output from a computation at the principal node must be sent to the local node where it is stored for high speed output to the graphics terminal. The user then uses the terminal to produce various graphical representations of the data. As he scans through his results, he can quickly make hard copies of those pictures he finds most interesting or generate different, more informative, representations of the data based on the results that were actually generated by the computation. The goal is a deeper understanding of the physics and the elucidation of the most promising ideas for subsequent computations and investigations."

- Press Report, p. 32-33

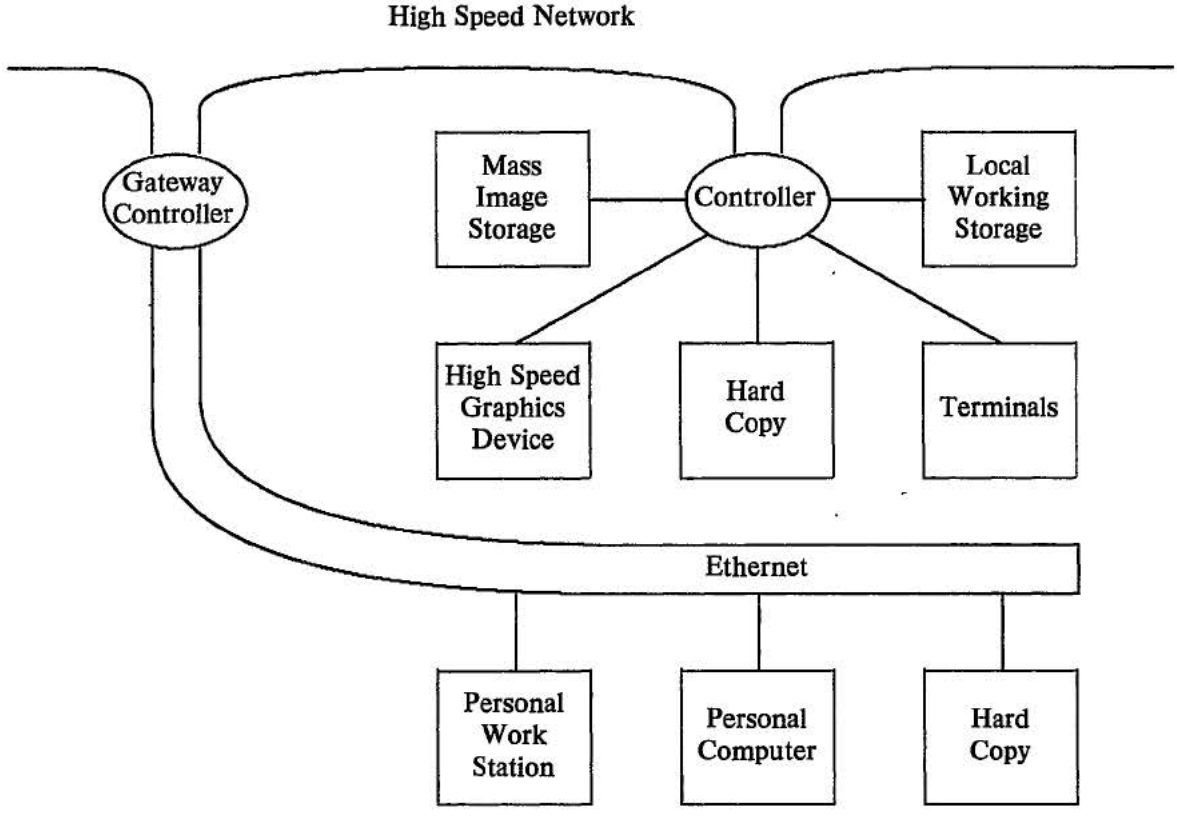


Figure 4: Local Node

The major additional features our local nodes have over those suggested in the Press Report are in the areas of high resolution graphics and in personal work stations. The capacity of a supercomputer is so great that the storage required to document a hydrodynamics or engineering simulation run can be enormous. Rather than bog down the Central Mass Store and the network everytime a researcher wants to view his images, we will establish high volume mass storage facilities at those local nodes whose research requires them. By 1985, we anticipate that terabit capacity will be available on laser disk "jukeboxes." Each laser disk can hold about 10 gigabits and a "jukebox" will contain up to 100 disks. These jukeboxes will serve as image archives for a local node. High-throughput graphics devices (e.g. CAD/CAM work stations) will be available on these sites for viewing and manipulating these high resolution displays (1280 x 1024 pixels, 24 bits deep) at movie speed. These specialized devices have a number of internal processors just to handle graphics, but they must be driven by a high speed super-minicomputer which serves as the controller for the local node (Figure 4).

We intend that all major users of the supercomputer enter the network from a "smart" work station. We anticipate two levels of work stations, one based on the Motorola 68000 family of processors like the SUN or the APOLLO, and a less powerful station based on an enhanced IBM personal computer. Prototypes of the former are already being tested at LLNL in the CTSS environment, while the latter are already in experimental use at LANL and NMFECC. We plan to install 24 initially and another 12 in each of the second and third years. This enhancement will present a high-usability access for both editing and graphics output. In addition to off-loading routine tasks from the supercomputer, we believe most scientists and engineers will find these work stations indispensable for everyday work. They will have symbolic manipulation packages like MACSYMA or SMP, ordinary differential equation solvers, word processing and drafting capabilities, etc. Also, their graphics capabilities will be outstanding. They will be hooked together in clusters by Ethernet which is in turn connected to the network through a Gateway and File Server. The operating system will be UNIX which provides very sophisticated tree-structured files and network communications. Many specialized processor boards are now becoming available on MULTIBUS for such work stations. These work stations plus processor boards have the power of superminicomputers at a fraction of the cost.

Both of the above innovations in image processing and work stations are fairly simple to plan, with the principal difficulty lying in deciding how long to wait before making a selection. The choice of work stations is improving dramatically, in both price and capability, so we wish to withhold a selection as long as possible. A major development that we expect to occur is the active combining of these new technologies to further improve presentation of complex results to users. For example, large storage, a fast network, and a good quality display, will allow us to develop tools that accumulate many raster pictures and then present them as a movies under the user's direction. Alternatively, the combination of video tape with a video grade cable system allow development of mixed video/digital work stations attacking the same problems. We plan to pioneer this method of increasing research productivity at Illinois.

V.C.4. Mass Storage

It is essential to have a large capacity hierarchical mass storage facility to store the enormous volume of files generated by users of a supercomputer. This will hold the permanent files as opposed to the temporary files which are stored on the supercomputer's disk farm shown in Figure 2. Lack of such a facility is one of the major productivity bottlenecks in many underconfigured supercomputer installations.

Fortunately, Los Alamos seems to have solved this difficult problem in its Common File System (CFS - see COMPCON SPRING, February 1982 for details). A schematic diagram of the facility is shown in Figure 5. The controllers are IBM 4341 level machines which run the CFS programs with no modification to the IBM operating system. Several such machines are already at Illinois and will be used to provide redundancy for the one machine funded by this proposal. This CFS software has been exported to other installations already. Active files are kept on disk but are migrated to cartridge if they have not been accessed recently or if they are too large. After an even longer time, the cartridges are placed offline. The following table, adapted from the COMPCON article, shows that while most accesses are to disk, they contain but a small fraction of the storage capacity. Most files are off-line or on the cartridge mass storage devices. Access times are very short, a key feature for us in our proposed high productivity system.

Device	File Type	Total Storage Capacity	% of total storage	% of access	access time
3350 Disk	Active	6×10^9 Bytes	1	85	5 sec
3850 Mass Storage Device	Less Active Larger	3.5×10^{11} Bytes	19	14	1 min
Off-line cartridge storage	Inactive	unlimited	80	1	5 min

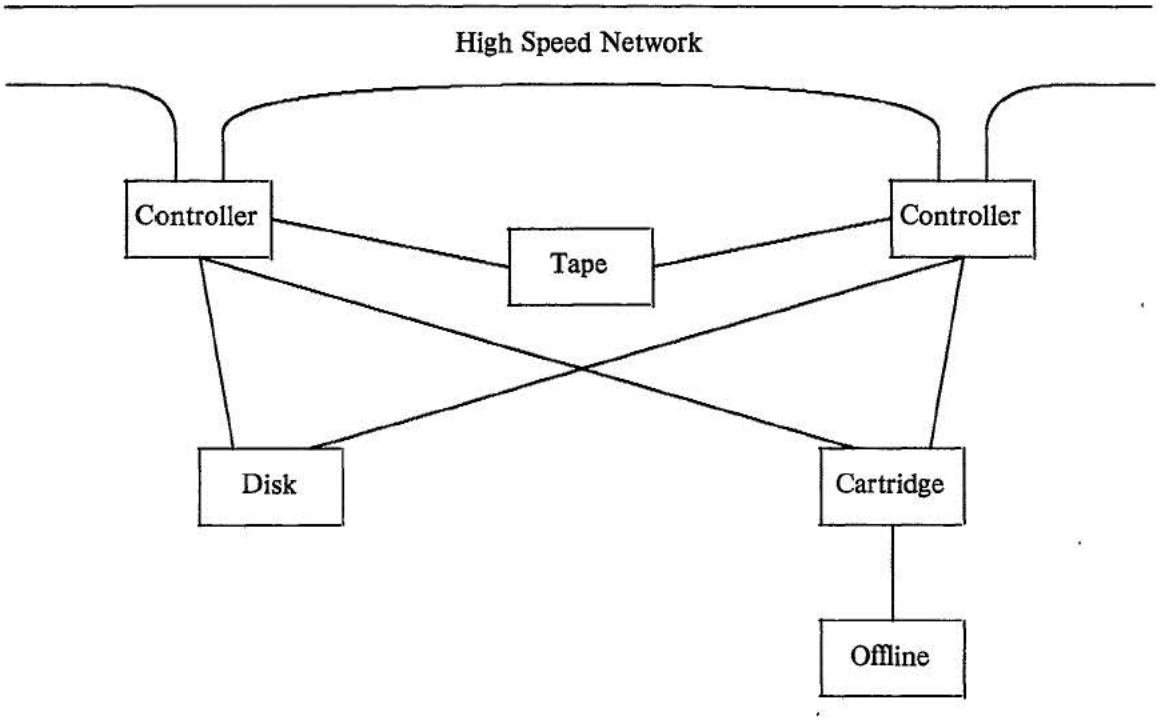


Figure 5: Mass Store System

The Los Alamos CFS supports CTSS, NOS, and VMS timesharing systems. In addition, CFS works under a limited UNIX and with intelligent work stations. The system is very fast and reliable and should be capable of handling the volume of data our system produces during its lifetime. Because computer staff at Illinois are already using IBM 4341 computers and are developing a mass store facility for the campus computer system, we should find it very easy to work with Los Alamos in installing this subsystem at an early stage of development. We are proposing that this grant support the expansion of the existing Illinois file subsystem to handle the traffic caused by the supercomputer. By the time this subsystem is installed we anticipate that this service will already be available to other CSO and dedicated computers. This budget item therefore represents a share, rather than the full cost of this service.

V.C. 5 Central Output Facility

Finally, our system will require a high throughput centralized output facility (see Figure 6). Experience at the national labs has shown that paper cannot be the standard output medium for a supercomputer. Microfiche is the standard for most numerical and graphical archiving. Slides (35mm) and movie film (16mm) are also used extensively. Laser printers and high speed plotters of various sizes are used for line graphics and numerical tables which the user wishes to have at normal size. All of these devices must be very fast, if they are to keep up with the supercomputer.

It seems likely that we will import the PAGES output system from Los Alamos National Laboratory. This system is built around a VAX controller running the PAGES software, FR-80 or Dicomed film output devices, and laser printers. The volume of output of a major integrated supercomputer facility is enormous. For instance, the daily production of LANL, with about twice our projected supercomputer power is:

1800	microfiche (150,000 frames daily)
3000	35mm slides
6000	16mm movie frames
40,000	printed pages
400	11" plots
75	36" plots

This throughput requires four film output devices and two laser printers. Our facility will have only one of each and will be shared with the main campus computing load, as will the costs.

The production of movies will be automated on both film and video tape. Standardized software will be provided so that users will only have to submit a file of images and the resulting movie will be available within a day. Animation controllers for both film and video tape are already available for purchase. Of course, many low volume versions of these hard copy devices will be available at the local nodes for "quick-look" at intermediate results. The output at the centralized facility will be of archival and publishable quality.

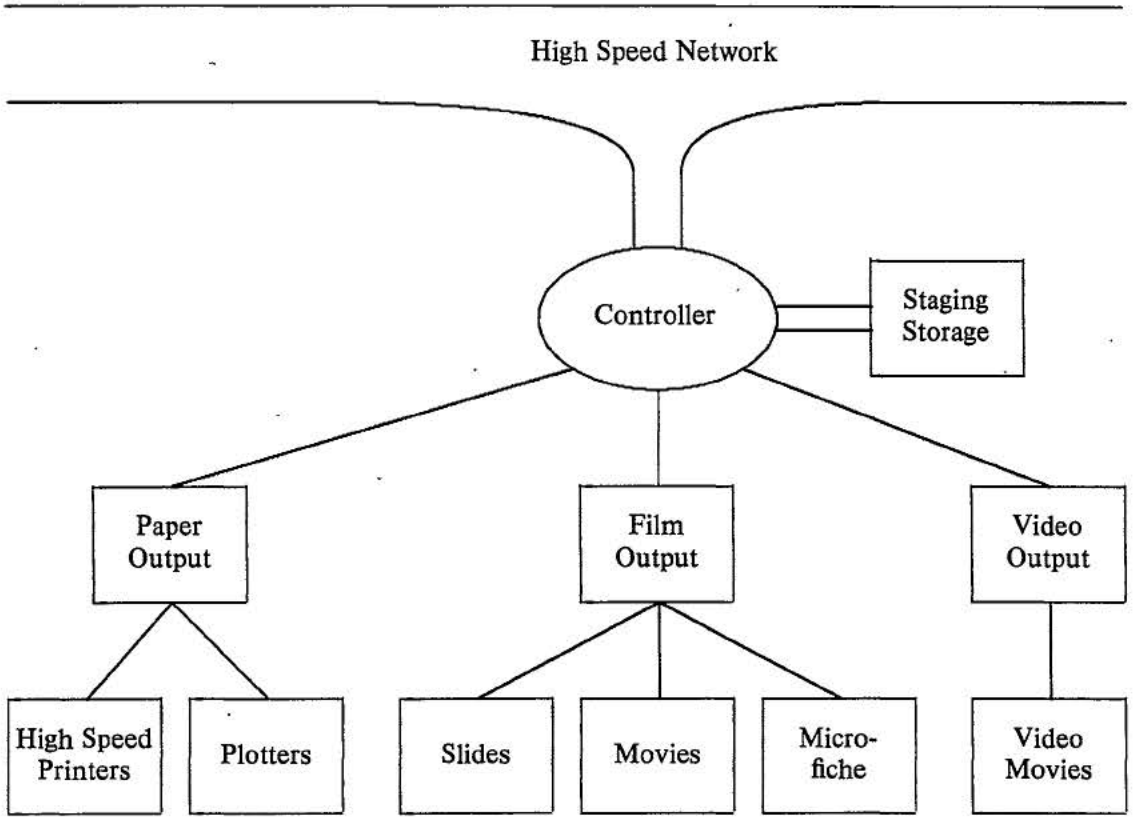


Figure 6: Centralized Output Facility

V.D. Staffing

The staffing plan for this project is crucial to its success. Because it represents a major recruiting effort, we will take two simultaneous approaches. First, we will start a national recruiting effort aimed at senior positions. In these the emphasis will be on experience with supercomputers, advanced workstations and numerical analysis. Second, we will recruit in the rich local environment for junior staff who can begin some tasks and training immediately. Our objective for filling positions is:

By month 6 after approval

Scientific Director
Project manager (Associate Director)
Business manager
Senior communications person
One documentation person
One senior and one junior systems programmer
Three senior and three junior systems consultant
One senior numerical consultant and librarian
One graphics programmer
Operations supervisor
Two clerical persons
Electronic technician
One vendor supplied analyst

By arrival of system - approximately month 12

Junior communications person
Numerical consultant
Three graphics programmers
Senior workstation programmer
Eight operations staff
Electronics technicians

By month 36 we will fill the remaining positions.

The early recruits will be primarily involved in making the system operational, setting up initial support services, and integrating things into the network. By having them for about six months prior to the initiation of service, we can provide a period of training, as well as involving them in the detailed decisions that will be important, but must be made early. The final level of staffing, thirty-two professional and eleven operational and four administrative, will provide for very adequate support of routine operations plus a modest development staff on specific projects.

In the building process there will be some use of existing CSO staff, particularly in areas such as using existing systems as a means of access, use of the Hyperchannel and broadband cable systems, and assistance with recruiting. In addition to the staff directly associated with the project, its placement in a university means that a wide variety of research interests will generate efforts involving graduate students. Examples of such research could include networking, workstations and other obvious topics. On the other hand it could include such diverse topics as human factors (Psychology and Industrial Engineering).

BUDGET AND SCHEDULES

The overall budget is shown along with a manpower schedule and a breakdown of the components of the central computer. This budget represents the five year growth into a fully operational, fully configured facility.

Each of the major elements of the budget is justified in Part V. Equipment and its maintenance is the largest item, divided between the central computer and support equipment. Personnel costs represent about thirty percent of the fifth year budget.

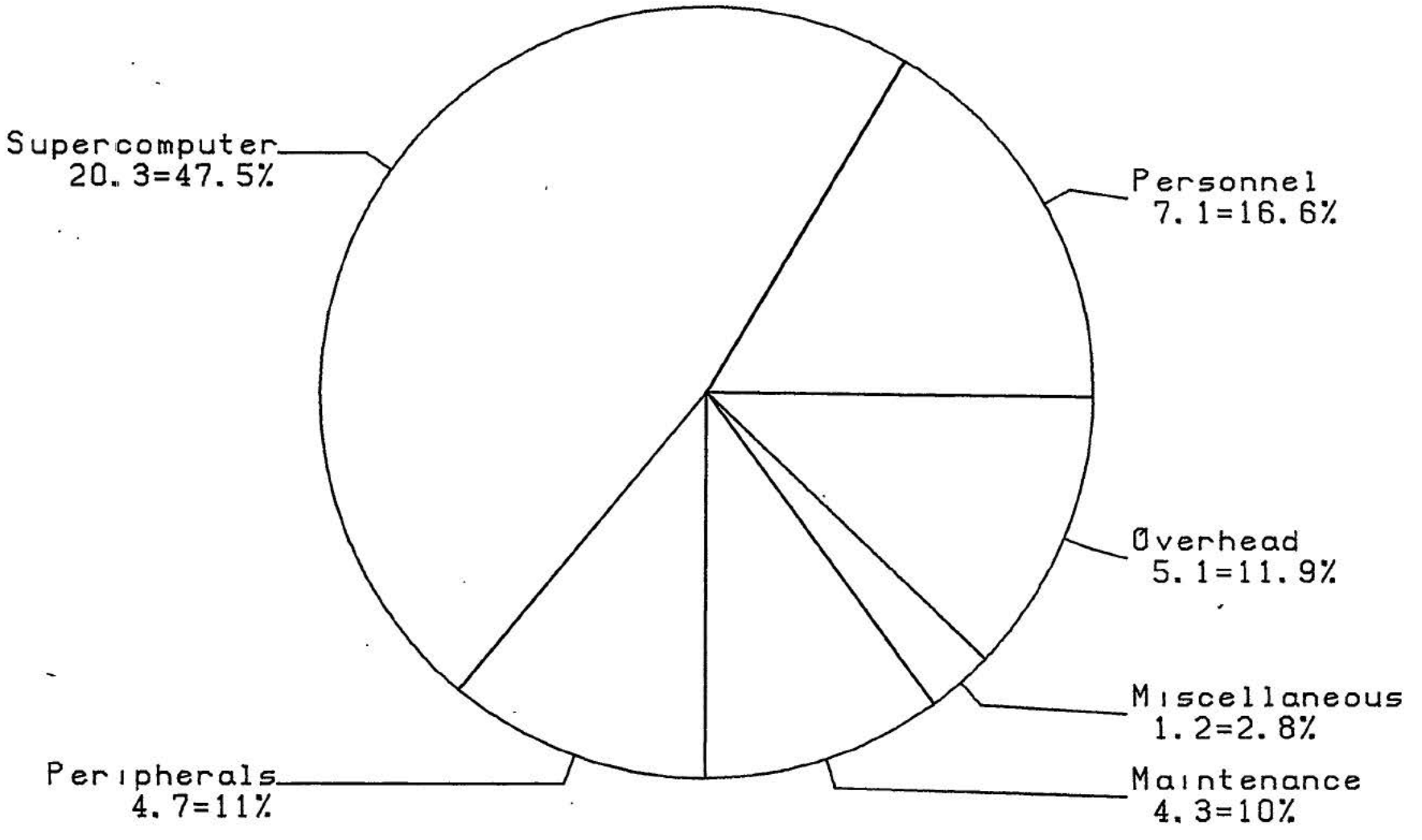
The University plans to provide additional support, beyond that sought in this proposal from NSF. The value of the University support will be approximately eight percent of the NSF total requested. This University support will be made in direct funding plus machine room space, power and other support not included in either the NSF request or in the overhead on MTDC. In addition, the University will provide personnel support by Computing Services Office staff, and release faculty time, equivalent to one FTE for committee work. This latter cost-sharing is estimated as a $200,000 per year. Thus, the total University contribution will exceed ten percent of the amount requested from the NSF. The total University commitment will be focused towards (1) renovation of machine room and office space for project staff (2) the salary of the scientific director (3) the visitors program (4) staff recruiting costs (5) additional equipment and supplies and (6) additional staff training.

The University is already actively seeking industrial grants to enrich the campus computing environment. The proposed Center should attract much greater support from those sources, because it will provide a national showcase for their products.

We wish to move rapidly to an operational state, therefore we plan to overlap a great deal of planning activity with this proposal's review process. For example, the study of available equipment alternatives, for at least initial subsystems, will take place during this time. We estimate that two FTE of professional staff will be devoted to this. This additional expense is also being borne by the University. In summary, we believe the University of Illinois is making a strong across-the-board financial commitment to the Center.

PERSONNEL	Year 1	Year 2	Year 3	Year 4	Year 5	TOTAL
Staff (Schedule 1)	403,000	1,094,000	1,483,000	1,603,000	1,766,000	6,349,000
Fringe Benefits (12.535%)	51,000	137,000	186,000	201,000	221,000	796,000
TOTAL DIRECT SALARIES and Benefits	454,000	1,231,000	1,669,000	1,804,000	1,987,000	7,145,000
EQUIPMENT						
Supercomputer System (Schedule 2)	4,050,000	4,050,000	4,050,000	4,050,000	4,050,000	20,250,000
Hyperchannel expansion	500,000					500,000
Mass storage system	200,000	200,000	200,000	200,000	200,000	1,000,000
Printing and microform	200,000	200,000	200,000	200,000	200,000	1,000,000
Workstations and communications	250,000	250,000	250,000	250,000	250,000	1,250,000
Enhancements	0	250,000	250,000	250,000	250,000	1,000,000
Contract Maintenance	738,000	821,000	866,000	911,000	960,000	4,296,000
TOTAL EQUIPMENT	5,938,000	5,771,000	5,816,000	5,861,000	5,910,000	29,296,000
MISCELLANEOUS						
Supplies (Disk packs, paper, film etc).	40,000	80,000	90,000	100,000	110,000	420,000
Software (Hyperchannel, graphics engineering packages)	30,000	60,000	60,000	60,000	60,000	270,000
Travel for Committees (Incl. Honoraria)	20,000	20,000	20,000	20,000	20,000	100,000
Annual conference expenses	0	25,000	25,000	30,000	30,000	110,000
Staff Travel	35,000	35,000	35,000	40,000	40,000	185,000
Education	5,000	5,000	5,000	5,000	5,000	25,000
TOTAL MISCELLANEOUS	130,000	225,000	235,000	255,000	265,000	1,181,000
TOTAL DIRECT COST	6,522,000	7,227,000	7,720,000	7,920,000	8,162,000	37,551,000
Exempt Items	5,210,000	4,985,000	4,985,000	4,995,000	4,995,000	25,170,000
TOTAL Modified Direct Cost Base	1,312,000	2,242,000	2,735,000	2,925,000	3,167,000	12,381,000
Overhead at 42% MTDC	551,040	941,640	1,148,700	1,228,500	1,330,140	5,200,020
GRAND TOTAL	7,073,040	8,168,640	8,868,700	9,148,500	9,492,140	42,751,020

TOTAL BUDGET $42.7 MILLION
Breakdown by Category in Millions of Dollars

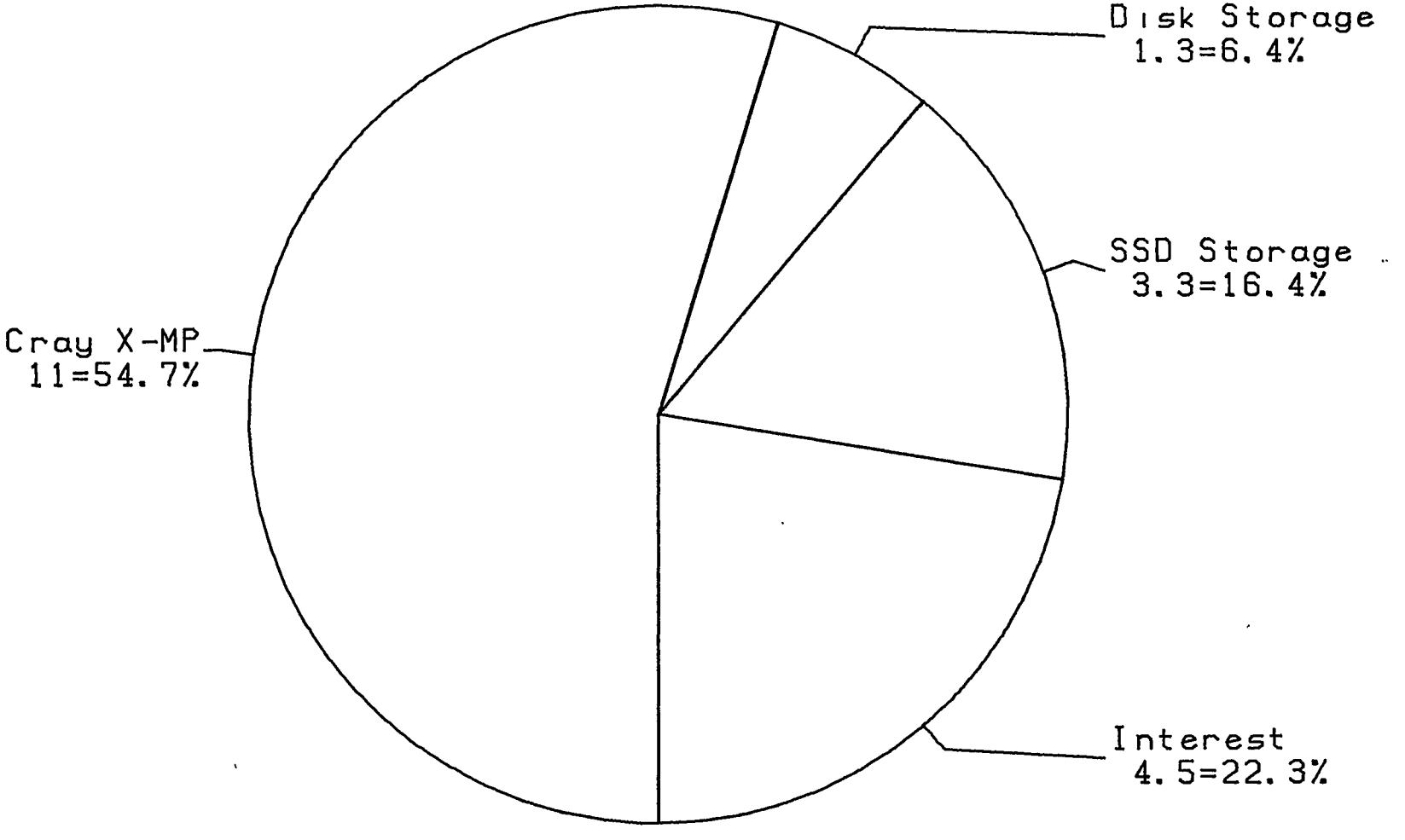


Schedule 2 (Supercomputer Purchase)

1 X-MP/24 (2 processor, 4MW)	11,000,000
4 DCU-4 Disk Controller	240,000
16 DD-29 Disk Unit	1,119,200
2 FEI-1 Front End	72,000
1 Solid State Disk (32 MW)	3,280,000
1 High Speed (1250) MB Channel	60,000
TOTAL PURCHASE	15,771,200

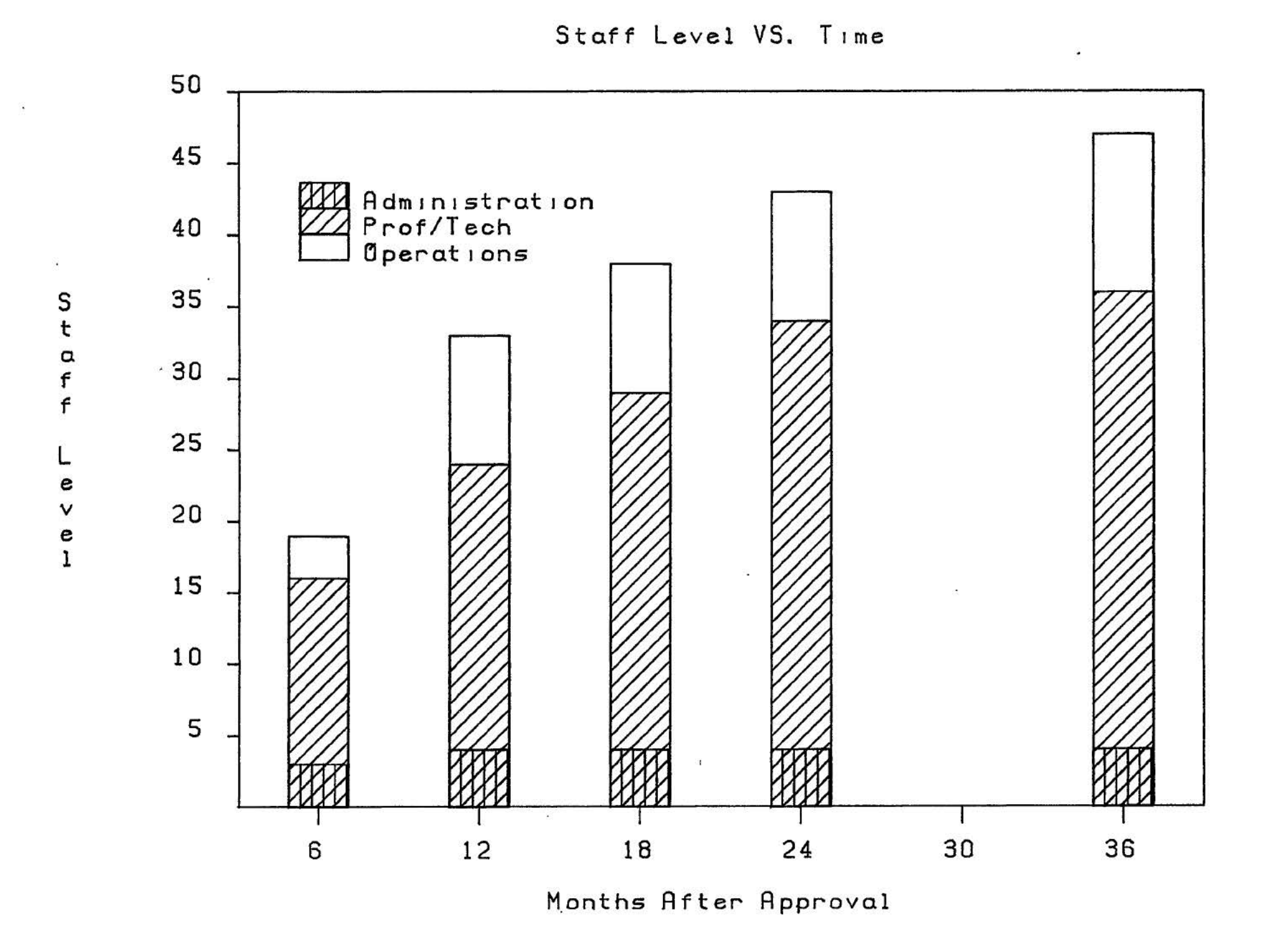
The total purchase (including interest) will be divided into five equal payments of $4,050,000 over a five year period. (See Budget)

SUPERCOMPUTER $20.25 MILLION
Breakdown by Components in Millions of Dollars



Schedule 1 (Personnel)

	YEAR 1		YEAR 2		YEAR 3		YEAR 4		YEAR 5	
POSITION	Months	Cost	Months	Cost	Months	Cost	Months	Cost	Months	Cost
Scientific Director	6	0	6	0	6	0	6	0	6	0
Manager (Associate Director)	9	34,000	12	49,000	12	52,000	12	57,000	12	61,000
Business Manager	6	19,000	6	20,000	6	22,000	6	24,000	6	26,000
Senior Systems Programmer	9	33,000	36	142,000	36	154,000	36	166,000	36	180,000
Junior Systems Programmer	12	27,000	36	87,000	48	126,000	48	136,000	60	182,000
Senior Communcations Analyst	6	24,000	12	52,000	12	56,000	12	61,000	12	66,000
Junior Communications Analyst	0	0	12	29,000	12	31,000	12	34,000	12	37,000
Electronic Technician	12	24,000	24	52,000	24	56,000	24	60,000	24	65,000
Senior User Consultant (Systems)	18	54,000	36	117,000	48	168,000	48	182,000	48	196,000
Junior User Consultant (Systems)	18	36,000	36	78,000	36	84,000	36	90,000	36	99,000
Senior User Consultant (Numerical)	9	29,000	27	95,000	36	136,000	36	147,000	36	159,000
Senior Graphics Programmer	9	29,000	18	63,000	24	90,000	24	98,000	24	106,000
Junior Graphics Programmer	6	14,000	15	37,000	24	63,000	24	68,000	24	73,000
Workstation Programmer	0	0	18	60,000	48	168,000	48	182,000	48	196,000
Documentation Editor	9	15,000	18	34,000	24	49,000	24	52,000	24	56,000
Operations Supervisor	12	20,000	12	22,000	12	24,000	12	26,000	12	28,000
Operations Staff	24	30,000	96	130,000	120	174,000	120	188,000	120	202,000
Clerical Staff	15	15,000	24	27,000	24	30,000	24	32,000	24	34,000
Total Direct Cost		**403,000**		**1,094,000**		**1,483,000**		**1,603,000**		**1,766,000**


Staff Level VS. Time
Administration
Prof/Tech
Operations
Staff Level
50
45
40
35
30
25
20
15
10
5
6
12
18
24
30
36
Months After Approval

PROJECT MILESTONES

A set of initial target dates has been outlined below. These assume the project is funded about April 2, 1984, and that some money is made available in FY84.

Presently available staff from CSO and several faculty members will carry out initial studies, during the grant review process, so that many detailed decisions can be converted into orders upon notification of approval. Changes in approval data will materially effect these schedules. Of particular importance is the staffing process, since no major activities can be undertaken before the staff is available and trined. The ability to meet these schedules will be dependent on achieving the desired staffing levels on time.

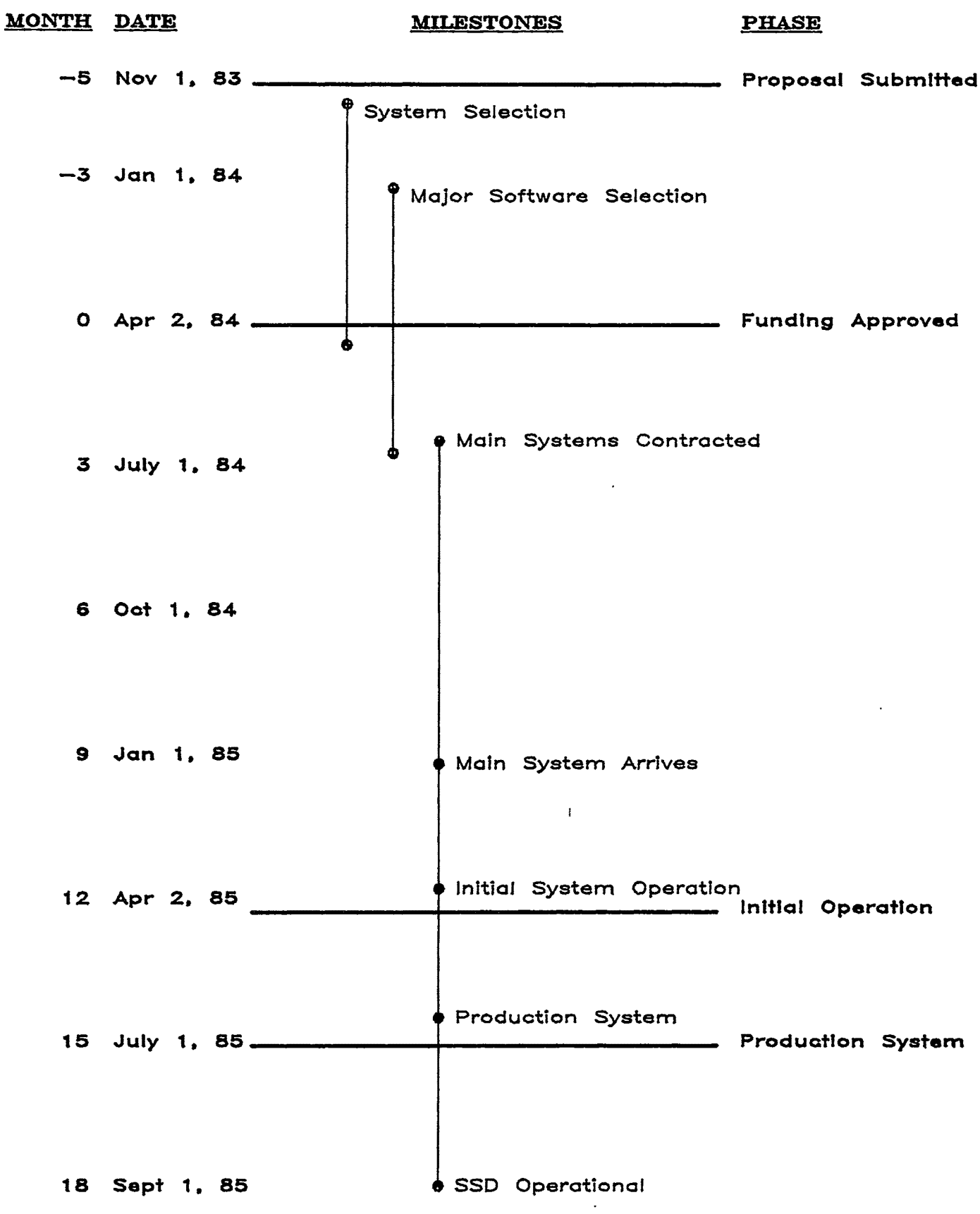
The initial areas of concentration will be acquiring and bringing into service a basic system, allowing job submission from familiar systems, interconnection ot the Hyperchannel network, and starting a basic consulting service. As staff become available work will expand into the areas of workstation access, output graphics, and more extensive consulting. Some rough requirements for manpower on major tasks are estimated. Each new staff member is likely to require a three month period of study, as well as a one month training program before becoming effective.

MAJOR TARGET DATES

DATE	PROJECT MONTH	OBJECTIVE	MAN-MONTHS
11/83	- 5	Proposal submitted	
12/83	- 4	Start detailed study supercomputer choice	3
1/84	- 3		
2/84	- 2	Start detailed study supercomputer software	3
		Organize selection of subsystem hardware	1
		Schedule vendors, gather technical info	1
3/84	- 1	Detailed study for mass store subsystem	3
		Hyperchannel plan	1
		Set up recruiting plan	2
		Plan renovation	3
4/84	0	Funding approved	-
5/84	1	Start recruiting	1
		Start renovation	2
		Order mass store subsystem	-
6/84	2	Select supercomputer	2
7/84	3	Have operating system selected	-

8/84	4	New staff begin to arrive	-
		Contracts for supercomputer	1
		Begin studies and implementation of:	
		Initial access method	6
		Initial output systems	6
9/84	5	-	-
10/84	6	Install Hyperchannel expansion	6
		Mass store arrives	-
11/84	7	Hyperchannel - VIP/VMS	1
		Begin workstation network	6
12/84	8	Mass store to IBM/VM	3
		Mass store to CDC/NOS	3
1/85	9	Renovation complete	-
		Major staff training	12
2/85	10	Processor arrives	-
		Install operating systems	8
3/85	11	Hyperchannel to system	2
4/85	12	Basic system operational	-
		Short course for users	2
5/85	13	Mass store to supercomputer	3
		Consulting service begins	
6/85	14	Simple workstation operating	3
7/85	15	Production system	
10/85	18	Solid state swapping/files	6
4/86	24	Measure system productivity	6
		Order productivity enancements if necessary	

SYSTEM MILESTONES



MASS STORE MILESTONES

MONTH	DATE	MILESTONES	PHASE
−5	Nov 1, 83		Proposal Submitted
−3	Jan 1, 84		
		Select and Order Mass Store	
0	Apr 2, 84		Funding Approved
3	July 1, 84		
6	Oct 1, 84	Arrives	
		Mass Store on IBM/CDC	
9	Jan 1, 85		
12	Apr 2, 85		Initial Operation
		Mass Store on Supercomputer	
15	July 1, 85		Production System
18	Sept 1, 85		

COMMUNICATIONS MILESTONES

MONTH	DATE	MILESTONES	PHASE
−5	Nov 1, 83		Proposal Submitted
		• Initial Hyperchannel Operational IBM/CDC	
−3	Jan 1, 84		
0	Apr 2, 84		Funding Approved
		• Renovation of Machine Room Including Power and A/C	
		• Extend Hyperchannel DCL—Astronomy For Supercomputer and VIP	
3	July 1, 84		
6	Oct 1, 84		
		• VIP Operational on Hyperchannel	
9	Jan 1, 85		
		• Main System Arrives	
12	Apr 2, 85		Initial Operation
15	July 1, 85		Production System
18	Sept 1, 85		

APPENDIX A

GROUP I USERS

RESEARCH PROPOSALS

Proposals for the first group of users (see Section IV - Scientific and Engineering Supercomputing) are included in this appendix. Faculty members in this group intend to make immediate use of the proposed supercomputer. A summary of the faculty, their research areas, their students and collaborators at other institutions, their current computer usage and their projected first-year usage of the proposed supercomputer can be found in Table 2 in Section IV. Projected computer usage is given in CRAY-1 equivalent hours, and it is assumed that 12,000 equivalent hours per year will be available on the proposed supercomputer because of the multiprocessor architecture (two CPU's assumed).

RELATIVISTIC ASTROPHYSICS

Larry Smarr - Associate Professor

Departments of Astronomy and Physics

Smarr and his colleagues use supercomputers to solve for multi-dimensional dynamical solutions of the basic equations of classical physics. These equations include those governing general relativity, hydrodynamics, magnetohydrodynamics, and the collisionless Boltzmann equation. Special demands are made on a supercomputer facility in carrying out such a scientific research program. Instant access to graphical representation of the solutions is essential. At a given time in the evolution, up to 40 quantities, in several spatial dimensions, must be scanned to assure that a reliable solution is being computed. Multicolor images are necessary to bring out the physics of the resulting flows. Fast turnaround (minutes) of small and mid-sized jobs must be possible at all times. Typically, many hundreds of such runs are required in the process of developing a new code. Finally, high resolution runs require large fast core (megawords) and long times (10-50 hours). The output from such runs requires mass storage devices. Four major research areas are currently being investigated with supercomputers.

The solution of Einstein's equations of general relativity requires the simultaneous solution of many coupled elliptic and hyperbolic equations. These equations govern the curvature of spacetime itself and therefore the interpretation of the physics involves novel conceptual methods. Examples of problems that are being attacked are 1) the head-on collision of two black holes, 2) neutron star and black hole formation, and 3) gravitational radiation generation and propagation. Charles Evans, currently getting his Ph.D. under Jim Wilson at Lawrence Livermore National Laboratory (LLNL) and starting as Smarr's postdoc in Fall 1983, has perfected a code which solves the axisymmetric dynamic Einstein equations with a matter source term. Accurate runs currently take 10 hours on the CRAY-1 at LLNL. Because the solution space to these equations is completely unknown, we anticipate using up to 200 supercomputer hours per year, as soon as the Illinois supercomputer is available. Without a supercomputer at Illinois, Evans will be able to compute at LLNL with Wilson only every few months on trips to LLNL from Illinois. With a supercomputer that has a very large and fast solid state disk (SSD), Evans and Smarr will also be able to develop the first 3-D general relativity codes.

Another area of intense astrophysical interest is that of accretion onto compact objects, neutron stars and black holes. Graduate student John Hawley, Smarr, and Jim Wilson (LLNL) have developed codes which can calculate fully relativistic, rotating, magnetohydrodynamical flows in the strong gravitational fields of such compact objects. Shocks, vortices, and jets are common in these flows. Color movies have turned out to be crucial in visualizing the dynamics of these complicated solutions. This code has been given 30 hours during the summer of 1983 on the CRAY-1 at the Max-Planck Institute for Physics and Astrophysics in Garching near Munich, West Germany. By fall, the code will be fully vectorized and ready for production runs. Such runs will take from 2-10 hours on the CRAY. Therefore, we anticipate that this project will require up to several hundred supercomputer hours per year to explore this unknown physical arena.

Supersonic jets are being discovered in many different types of astrophysical environments from stellar formation to radio galaxies. A systematic study of the nonlinear formation and propagation properties of axisymmetric and slab symmetric jets has been undertaken by Smarr with Michael Norman and Karl-Heinz Winkler of the Max-Planck Institute. Using their CRAY-1A, high resolution solutions (50,000 grid points) were obtained which showed a variety of nonlinear persistent structures (repeated shocks, vortex shedding, Mach disk-triple point configurations, etc.), most of which have characteristic observational signatures. These numerical simulations are also of interest to laboratory experimentalists and industrial engineers who study or use supersonic jets. This project has already used at least 600 CRAY-1 hours over the last two years. We hope to have Norman and Winkler as visitors to Illinois as soon as the supercomputer arrives. The 2-dimensional jet studies will require at least 400 hours during the first year. We will also develop, using the SSD, a fully 3-D code (5 million grid points) to model the observed nonlinear helical instabilities of these jets. Each high-resolution 3D run, using state of the art finite differncing techniques will require several hundred hours/run. That program alone could easily use 1000 supercomputer hours in the second year.

Joan Centrella has been a postdoctoral fellow in Smarr's group during the last two years and will be at the University of Texas starting Fall 1983; she has pioneered the use of supercomputers to study structure in the early universe. The possibility of new massive elementary particles (neutrino, photino, gravitino, etc.) has caused a great deal of excitement in cosmology. It seems likely that the dynamics of the universe is controlled by this unseen matter. Centrella and Adrian Melott (Department of Physics and Astronomy, University of Pittsburgh), are studying the large scale structure which develops in this dark matter as the universe expands. They use a three-dimensional cloud-in-cell code to follow the evolution of this self-gravitating but collisionless matter. They find that an interacting cellular structure forms on scales of superclusters with large voids between filament and pancake-like concentrations of the dark matter. Centrella and co-workers are now "reading out" the quantities which can be compared with observational data. These calculations were run at LLNL and are going to be run on the CRAY X-MP at Cray Research. This code will then be available for use on the Illinois supercomputer when it arrives. Besides refining the above calculations, Centrella will be collaborating with Evans and Smarr on developing a 2-D general relativistic cosmology code. Again, probably 100-200 supercomputer hours will be used in the first year.

Several themes run through all this work. First, analytic methods are useless for providing the solutions. In fact, they are often worse than useless at predicting the final state of highly non-linear systems, since the linearized behavior of the equations may be radically different than the non-linear behavior. The discovery of the rich phenomonology of solution space is relatively straight forward with supercomputers. The visualizations of these solutions often suggests fruitful new avenues of non-computer mathematical studies (e.g. solitons). Finally, the supercomputer provides a physics laboratory for studying the detailed structure of processes which cannot otherwise be studied experimentally or observationally.

I estimate that my group and collaborators have used over 200 hours of CRAY-1 time per year to solve the problems mentioned above. That time has been obtained at Max-Planck or LLNL. Our progress has been hampered by the fact that the collaborators can only get together a few times a year. The codes that we are running on the CRAY-1 now will transfer directly to the CRAY X-MP. As stated above, some 1000 CRAY hours per year could be used starting as soon as the supercomputer is available at Illinois. This work would be split between the four research groups mentioned above. We will be using the Parafrase program of the University of Illinois Laboratory for Advanced Supercomputers to optimize the vectorization of all our production codes.

Finally, for the first time, we can begin to attack fully 3-D high resolution flows (jets, gravitational collapse, and black hole collision). This is because of the large fast memory (32 megawords on the SSD) on the proposed supercomputer and because we could obtain substantial computer time. These multidimensional codes will employ state of the art numerical algorithms and take full advantage of the machine architecture. Even so, individual runs will require up to several hundred CPU hours. Thus by the second year our group could easily require several thousand hours.

References in Computational Astrophysics

(1) J. Centrella. "Interacting Gravitational Shocks in Vacuum Plane-Symmetric Cosmologies," Ap. J. *241,* 875 (1980).

(2) J. Centrella and R. Matzner. "Colliding Gravitational Waves in Expanding Cosmologies," Phys. Rev. D *25*, 930 (1982).

(3) J. Centrella. "Numerical Cosmologies," article in *The Origin and Evolution of Galaxies* , Proceedings of the VIIth Course of the International School of Cosmology and Gravitation, Erice (in press, 1982).

(4) J. Centrella and J. R. Wilson. "Collisionless Matter and Galaxy Formation," in *Energy and Technology Review* (March, 1983).

(5) J. Centrella and J. R. Wilson. "Planar Numerical Cosmology I: The Differential Equations," (Ap. J.,

in press, 1983) (University of Illinois Department of Astronomy preprint IAP 82-31).

(6) J. Centrella and J. R. Wilson. "Planar Numerical Cosmology II: The Difference Equations and Numerical Tests," preprint (1982). (University of Illinois, Department of Astronomy, Preprint IAP 83-11)

(7) J. Centrella and A. L. Melott. "Three Dimensional Simulation of Large Scale Structure in the Universe," Nature (submitted, 1983). (University of Illinois, Department of Astronomy Preprint IAP 83-6).

(8) D. Eardley and L. Smarr. "Time Functions in Numerical Relativity: I. Marginally Bound Dust Collapse," Phys. Rev., *D19*, 2239, 1979.

(9) J. Hawley and L. Smarr. "Numerical Models of Fat Disks: New Scenarios for Fluid Accretion into Black Holes," (University of Illinois Astronomy Department preprint IAP 83-14), to appear in *Numerical Astrophysics: A Meeting in Honor of Jim Wilson*, ed. J. Centrella.

(10) J. Hawley, L. Smarr and J. R. Wilson. "A Numerical Study of Nonspherical Black Hole Accretion. I. Equations and Test Problems," in press Ap. J. (University of Illinois Astronomy Department preprint IAP 83-9).

(11) J. Hawley, L. Smarr and J. R. Wilson. "A Numerical Study of Nonspherical Black Hole Accretion II. Finite Differencing and Code Calibration" in press to Ap. J. Suppl. (University of Illinois Department of Astronomy preprint IAP 83-13).

(12) J. Hawley and L. Smarr. "Black Hole Accretion: The Quasar Powerhouse" in *Energy Technology Review*, (March 1983).

(13) M. L. Norman, L. Smarr, J. R. Wilson, and M. D. Smith. "Hydrodynamical Formation of Twin-Exhaust Jets," Ap. J., *247*, 52, 1981.

(14) M. L. Norman, L. Smarr, K.H. Winkler, and M. Smith. "Structure and Dynamics of Supersonic Jets," Astron. & Astrophys., *113*, 285, 1982.

(15) M. Norman, K.H. Winkler and L. Smarr. "Propagation and Morphology of Pressure-Confined Supersonic Jets," Proceedings of the Torino Workshop on Astrophysical Jets, ed. Ferrari and Pacholczyk.

(16) L. Smarr. "Spacetime Generated by Computers: Black Holes with Gravitational Radiation," Ann. N.Y. Acad. of Sciences, *302*, 569, 1977.

(17) L. Smarr. "Gauge Conditions, Radiation Formulae, and the Two Black Hole Collision," p. 245, in *Sources of Gravitational Radiation*, ed. L. Smarr (Cambridge University Press, 1979).

(18) L. Smarr, C. Taubes, and J. R. Wilson, "General Relativistic Hydrodynamics The Comoving, Eulerian, and Velocity Potential Formalism," *Essays in General Relativity A Festschrift for Abraham Taub* ed. T. Tipler (Academic Press 1980).

(19) L. Smarr, J. R. Wilson, R. T. Barton, and R. L. Bowers. " Rayleigh-Taylor Overturn in Supernova Collapse," Ap. J., *246*, 515, 1981.

Recent Participation in Computer Panels

Smarr was a member of the NSF Press Committee on Computational Physics (1981). He wrote several appendices for the interagency Lax Report on Large Scale Computing in Science and Engineering (1982). He was one of the participants in the NSF workshop on Computer for Research, the results of

which were reported in the NSF Curtis report on a National Computing Environment for Academic Research (1983).

STELLAR EVOLUTION TYPE I SUPERNOVA SCENARIOS AND THERMAL PULSES IN AGB STARS

Icko Iben, Jr. - Professor

Head of the Department of Astronomy

Stellar evolution is a field in which almost every major advance has been associated with the advent of a new generation of faster and larger computers, a theme which I have formally explored on two previous occasions in *Computer Science and Scientific Computing,* ed. James M. Ortega (New York: Academic Press), 1976, p. 109 and in *Computers and Their Role in the Physical Sciences,* eds. S. Fernback and A. H. Taub (New York: Gordon and Breach), 1970, p. 595]. Currently, some of the most exciting work in the field is being done on supercomputers at Lawrence Livermore National Laboratory (LLNL) (Type II supernova explosions by Jim Wilson; Type I supernova explosions by Tom Weaver and Stan Woosley), at Los Alamos (Cepheid and hot white dwarf pulsations by Art Cox and John Cox; nova explosions by Sumner Starrfield and James Truran), and at the Max Planck Institute in Munich (supernova explosions by Dave Arnett, W. Hillebrandt, Ken Nomoto, and others).

Interestingly enough, the vital question as to how a star actually evolves into the Type I supernovae state has languished, for in many respects this question is both conceptually and numerically more difficult to answer than is the question of the explosion itself. We believe that Type I supernovae occur only as a consequence of mass transfer in binary systems, and yet a concerted effort to determine the most probable evolutionary scenarios which will lead to these events has not been made until recently (I. Iben, Jr. and A. V. Tutulov 1984, Ap. J., Suppl., February Issue). The steps through which appropriate systems pass may include:

(1) Common envelope stages, which produce a "bare" electron-degenerate dwarf made up of ^{4}He, of $^{12}C + {}^{16}O$, or of $^{16}O + {}^{20}Ne + {}^{24}Mg$ and bring the components closer together in preparation for a later mass transfer episode;

(2) Mass transfer stages brought about by Roche-lobe overfilling or wind ejection and capture. The Roche-lobe contact can be maintained by evolutionary changes or by angular momentum loss due to either a magnetic stellar wind or to the radiation of gravitational waves. Transfer can be on an evolutionary, a thermal, or a dynamic time scale;

(3) In the most likely case of two electron-degenerate dwarfs, a stage of dynamic mass transfer which results in the dissolution of one degenerate dwarf and the formation of a "heavy" disk and the subsequent leakage from this disk onto the remaining dwarf.

It is evident that there is a tremendous variety of possible paths that must be explored numerically, even after having narrowed down the list by applying general constraints as in the Iben-Tutukov paper. One of our major objectives is to pursue systematically all of these paths, beginning with those which have been already delineated as the most promising. The approach is very much akin to that followed by Appel and Haken in proving the four color theorem on University of Illinois computers in the mid-seventies. A modest pilot study has already been initiated on the University's Cyber machines.

Another major objective is to pursue the thermal pulse properties of asymptotic giant branch (AGB) stars. These stars consist of an electron-degenerate core, a helium- and carbon-rich zone, and a hydrogen-rich envelope. Hydrogen and helium burning phases alternate, thanks to a thermal instability which is triggered when the mass in the helium-rich zone reaches a critical value. During a pulse, fresh carbon and about 150 neutron-rich isotopes are produced. Under appropriate conditions of total stellar mass, electron-degenerate core mass, initial surface composition, etc., the newly produced isotopes are brought to the surface following each pulse. First, a stellar wind and then a planetary-nebula ejection event carry newly-made

isotopes into the interstellar medium and, we believe, play a significant role in the Galactic nucleosynthesis of these isotopes.

I have spent a major part of the past ten years studying these pulses and their consequences, initially using the National Center for Atmospheric Research and LLNL CDC 7600 computers and currently using the Cyber 174/175 computers at Illinois. It has become painfully clear that even 500 hours/yr on the Cyber machines is woefully inadequate to the task of obtaining a systematic understanding of how pulse and dredge-up characteristics depend on all of the relevant stellar parameters. Attempts to take shortcuts lead in many instances to physically unreasonable results. One simply has to pass, by *careful* brute force, through many, many pulses for many, many different cases. Access to a supercomputer at Illinois would make the task more reasonable and I estimate using about 600 hours of time during the first year it is here.

References

(1) I. Iben, Jr., "Cepheids, Presupernovae, and the ^{12}C (α,γ) ^{16}O Reaction." Ap. J., *178*, 433, (1972).

(2) J. Whelan and I. Iben, Jr., "Binaries and Supernovae of Type I." Ap. J., *186*, 1007 (1973).

(3) I. Iben, Jr., "Post Main Sequence Evolution of Single Stars." Annual Review of Astronomy and Astrophysics, *12*, 215, (1974).

(4) I. Iben, Jr., "Thermal Pulses; p-Capture, α-Capture, s-Process Nucleosynthesis; and Convective Mixing in a Star of Intermediate Mass." Ap. J., *196*, 525, (1975).

(5) I. Iben, Jr., "Neon-22 As a Neutron Source, Light Elements as Modulators and s-Process Nucleosynthesis in a Thermally Pulsing Star." Ap. J., *196*, 549, (1975).

(6) I. Iben, Jr., "Further Adventures of a Thermally Pulsing Star." Ap. J., *208*, 165, (1976).

(7) I. Iben, Jr., "Thermal Pulse and Interpulse Properties of Intermediate-Mass Stellar Models with Carbon-Oxygen Cores of Mass 0.96, 1.16, and 1.36 M_o." *217*, 788, (1977).

(8) James W. Truran and I. Iben, Jr., "On s-Process Nucleosynthesis in Thermally Pulsing Stars." Ap. J., *216*, 797, (1977).

(9) I. Iben, Jr., and James W. Truran, "On the Surface Composition of Thermally Pulsing Stars of High Luminosity and on the Contribution of such Stars to the Element Enrichment of the Interstellar Medium." Ap. J. *220*, 980, (1978).

(10) I. Iben, Jr., "Low-Mass Asymptotic Giant Branch Evolution. I." Ap. J. *260*, 821, (1982).

(11) I. Iben, Jr., and Alvio Renzini, "The Role of Semiconvection in Bringing Carbon to the Surface of Asymptotic Giant Branch Stars of Small Core Mass." Ap. J., *259*, L79, (1982).

(12) I. Iben, Jr., and Alvio Renzini, "On the Formation of Carbon Star Characteristics and the Production of Neutron-Rich Isotopes in Asymptotic Giant Branch Stars of Small Core Mass." Ap. J. *263*, L23, (1982).

(13) I. Iben, Jr., and Alvio Renzini, "Asymptotic Giant Branch Evolution and Beyond." Annual Review of Astronomy and Astrophysics, *21*, 271, (1983).

THEORY OF STAR FORMATION IN MAGNETIC INTERSTELLAR CLOUDS

Telemachos Ch. Mouschovias - Professor
Department of Physics and Astronomy

The formulation of a theory of star formation is a central problem in astrophysics. The formation of the solar system represents a special case of this problem. The notion that stars (of all kinds) form through the collapse and fragmentation of interstellar clouds dates back to the turn of the century. Yet the detailed physical processes that convert interstellar matter, of mean density 1 particle/cm^3 to stars, of mean density 10^{24} particles/cm^3, are still poorly understood. Once the density of a contracting cloud exceeds about $10^9 cm^3$, near hydrostatic equilibrium is reached, thereby introducing an enormous simplification in the problem. The physical processes occurring during the earlier, relatively diffuse stages of cloud contraction are fully dynamical, and it is here that our knowledge is particularly lacking. Forces due to gravity, thermal pressure, magnetic fields, rotation, cosmic rays, stellar photons and stellar winds are all comparable in magnitude. Thus, the diffuse interstellar medium is an extremely complicated physical system to understand and to model. However, its proper theoretical description is within the realm of nonlocal-thermodynamic-equilibrium magnetohydrodynamics.

Progress in understanding individual physical processes occurring in contracting interstellar clouds (invariably assumed to be nonmagnetic despite the observational and theoretical evidence to the contrary) has been significant (e.g., see reviews by Larson 1977; and Woodward 1978). Yet the results of such studies change not only quantitatively but also qualitatively when the magnetic field is properly accounted for (e.g., see reviews by Mestel 1977; Mouschovias 1978, 1981).

In a long-term project, we have undertaken to systematically decipher the role of magnetic fields in the formation of stars. After the initial work of Mestel and Spitzer (1956), Mestel (1965), and Spitzer (1968), progress in the field came to a standstill mainly because of mathematical complications. In a series of papers (see the 1981 review for precise references and a summary of each) in 1974 - 1976, we showed that the old problems could be formulated in fundamentally new ways, which allowed us to obtain detailed numerical solutions for such problems as the equilibrium and contraction of magnetic interstellar clouds. The theoretical predictions (e.g., of a relation between the magnetic field strength and the gas density in the core of self-gravitating clouds) stimulated significant observational activity which, in turn, induced new theorists to enter the field.

On the basis of semiquantitative arguments, we formulated in 1977 a scenario (to distinguish it from a complete theory) which a magnetic cloud will most likely follow on its way to giving birth to stars. Since that time, we have been attacking the major theoretical problems remaining unsolved in an effort to formulate a theory of star formation. The most severe of these problems is the so-called *Angular Momentum Problem.* It lies in the following. There is a minimum amount of angular momentum associated with any one interstellar cloud simply by virtue of its participation in the general galactic rotation. If this angular momentum is conserved during the contraction of a cloud, centrifugal forces will stop the contraction at densities many orders of magnitude smaller than typical stellar densities. Put differently, between two and five orders of magnitude of angular momentum must be lost if stars, ranging from wide binaries to single, are to form. In the years 1978-1980, we (with ex-graduate student E. V. Paleologou, in some papers) showed through exact, but (of necessity) idealized analytical calculations that frozen-in magnetic fields can resolve the angular momentum problem irrespective of whether the field is parallel or perpendicular to the axis of rotation. In both cases, but with different efficiencies, the magnetic field transports a sufficient amount of angular momentum from the cloud to the surrounding intercloud medium in a short enough time.

The interstellar magnetic field, having resolved the angular momentum problem, poses itself a serious problem in star formation: the magnetic flux of an interstellar blob of mass comparable to a stellar mass is typically four orders of magnitude larger than observed fluxes of even magnetic stars. Clearly, the field itself must decouple from the matter at some stage. During the last two years we have worked on this problem analytically and numerically. In the formulation and solution of an admittedly idealized problem (Mouschovias and Paleologou, 1981), we showed that the process of *Ambipolar Diffusion* (i.e., the diffusion of ions and electrons, carrying the field with them, through the neutrals) may resolve this *Magnetic Flux Problem.* The conclusion is not definitive in that the analytical approach limits us to rather idealized

geometries. We have, however, developed new numerical techniques which have allowed us to follow the collapse of a magnetic cloud while ambipolar diffusion is in progress. Our code is a *two-fluid magnetohydrodynamic* one. The more than 100 hours of Cyber 175 time expended in less than six months allowed us to obtain significant results using this code but in a one-dimensional application. We found that the flux in the core of a collapsing cloud decreases by more than four orders of magnitude in less than a million years, indicating that the process of ambipolar diffusion may indeed resolve the magnetic flux problem. For a definitive statement, two- and three-dimensional calculations are necessary.

The two-dimensional problem can be solved on the Cyber only if more than a few thousand hours of time are available. This constraint by itself will delay the solution of the problem by years. An attack on a realistic three-dimensional problem can only be undertaken locally if the Cyber is virtually dedicated to this problem. For this reason, an essential problem in the context of a theory of star formation cannot be addressed. The possible arrival of a supercomputer changes matters considerably. Presently impossible problems become feasible almost overnight, and currently very long-term projects can be completed in only a few years.

Until recently, we intended to make only a start on the attack of the self-consistent problem of a collapsing, rotating cloud in which ambipolar diffusion can progress in a manner consistent with the local state of ionization. Local availability of a supercomputer not only makes an attack on this central problem of star formation feasible, but also will lead to some solutions within a few-year time scale.

Ultimately a theory of star formation must predict the initial (stellar) mass function. For this it is necessary to study fragmentation in a *collapsing, rotating, magnetic* cloud. New numerical techniques will be necessary for an attack on this inherently three-dimensional problem and a superfast computer with enormous storage capability will be required. A supercomputer can handle this problem, but only if substantial time were available, perhaps as much as 1000 hours.

Aside from the new projects that the presence of a supercomputer will make feasible, the necessary computing (particularly at the code development stage) can be done all year round, while we also discharge our teaching and other responsibilities. Otherwise, we are restricted to doing this type of research during the summer months at national centers in the U. S. or in foreign countries. This will, in addition, allow us to better train our graduate assistants in advanced numerical techniques and code development necessary for their later professional success in solving astrophysical gas dynamical problems.

References

Larson, R. B. 1977, in *Star Formation* , eds. T. deJong and A. Maeder (Boston: Reidel), pp. 249-267.

Mestel, L. 1965, Quart. J. Roy. Astron. Soc., *6*, 161, 165.

Mestel, L. 1977, in *Star Formation,* eds. T. de Jong and A. Maeder (Boston: Reidel), pp. 213-232.

Mestel, L. and Spitzer, L., Jr. 1956, M.N.R.A.S., *116* , 503.

Mouschovias, T. Ch. 1974, "Static Equilibria of the Interstellar Gas in the Presence of Magnetic and Gravitational Fields: Large-Scale Condensations", Ap. J., *192* , 37.

Mouschovias, T. Ch. 1976, "Nonhomologous Contraction and Equilibria of Self-Gravitating, Magnetic Interstellar Clouds Embedded in an Intercloud Medium: Star Formation. I. Formulation of the Problem and Method of Solution", Ap. J., *206* , 753.

Mouschovias, T. Ch. 1976, "Nonhomologous Contraction and Equilibria of Self-Gravitating, Magnetic Interstellar Clouds Embedded in an Intercloud Medium: Star Formation. II. Results", Ap. J., *207* , 141.

Mouschovias, T. Ch. 1978, "Formation of Stars and Planetary Systems in Magnetic Interstellar Clouds," in *Protostars and Planets,* ed. T. Genrels (Tucson: Univ. of Ariz. Press), pp. 209-242.

Mouschovias, T. Ch. 1981, "The Role of Magnetic Fields in the Formation of Stars," in *Fundamental Problems in the Theory of Stellar Evolution,* eds. D. Sugimoto, D. Q. Lams, and D. N. Schramm (Boston: Reidel), pp. 27-59.

T. Ch. Mouschovias 1983, "Interstellar Magnetic Fields", *Advances in Space Research* , *2* , 71.

Mouschovias, T. Ch., and Paleologou, E. V. 1981, "Ambipolar Diffusion in Interstellar Clouds: Time-Dependent Solutions in One Spatial Dimension" 1981, Ap. J., *246* , 48.

Paleologou, E. V., and Mouschovias, T. Ch. 1983, "The Magnetic Flux Problem and Ambipolar Diffusion During Star Formation: One-Dimensional Collapse. I. Formulation of the Problem and Method of Solution", Ap. J., in press. (issue of Dec. 15).

Mouschovias, T. Ch., Palelogou, E.V., and Fiedler, R. A., 1983, "The Magnetic Flux Problem and Ambipolar Diffusion During Star Formation: One-Dimensional Collapse. II. Results", Ap. J., to be submitted.

Spitzer, L., Jr. 1968, *Diffuse Matter in Space* (New York: Interscience).

Woodward, P. R. 1978, A.R.A.A., *16* , 555.

COMPUTER SIMULATIONS FOR GAUGE THEORY AND ELEMENTARY PARTICLE PHYSICS

John B. Kogut - Professor
H. W. Wyld -Professor
John Stack - Professor
Michael Stone - Assistant Professor

Department of Physics

Dynamical calculations in relativistic quantum field theories were unheard of until the last few years. Many areas of elementary particle physics languished due to the lack of non-perturbative, systematic calculational methods. There were several reasons for this roadblock. First, the usual formulations of quantum field theory did not lend themselves to numerical investigation. This problem was partially solved by exploiting the similarity between statistical mechanics and field theory.[1] This equivalence led to space-time lattice formulations of relativistic field theory[2] and the application of statistical mechanics calculational methods, such as Monte Carlo simulations[3], to problems in elementary particle physics. Second, the huge number of degrees of freedom in field theories made precise analyses of realistic models seem impractical. The need for large space-time lattices to approximate continuum space-time made the problem particularly imposing. However, these pessimistic estimates vanished when computer simulations on SU(2) gauge theory were done on relatively small space-time lattices and several properties of a sensible, relativistic field theory were discovered. These included pioneering, first principles investigations into quark confinement[3] and spontaneous symmetry break.[4]

Many central problems in gauge theories of the fundamental interactions are now being studied by computer simulation methods. At this time no other systematic methods are known for this research. However, to do good calculations of this variety taxes the resources of the largest, fastest computers in the world. To simulate quantum chromodynamics one needs machines with central memories of several million words and speeds of several hundred megaflops. Access to substantial supercomputer time would have a significant impact on the development of non-perturbative calculations for gauge theories of strong interactions.

The high energy theory group at the University of Illinois has been active in this field for some time. The group includes Professors J. Kogut, J. Stack, H. W. Wyld, Assistant Professor M. Stone, two post-doctoral fellows and several graduate students. Significant results on quark confinement [5] (the heavy quark potential) and spontaneous symmetry breaking[4] (chiral symmetry) have been obtained by the group and many publications, review articles and summer school presentations have been made over the last few years. Recent work has required access to CRAY-1 machines and the group has worked closely with the Los Alamos National Laboratory in setting up university-based external user groups to run on its open system of three CDC-7600's and its CRAY-1A. The group is experienced in vector programming and the CRAY Time Sharing System (CTSS). It has advised other universities and funding agencies on supercomputer use extensively over the last year. It was recently awarded an external user account on the Magnetic Fusion Energy CRAY system for additional research. Several of its members will organize and contribute to the next Quark Matter Conference to be held in September at Brookhaven National Laboratory. Unfortunately, the scientific progress of the group is badly hampered by the limited supercomputer time available to theoretical physics through either the Los Alamos or MFE CRAY systems. Only tens of hours per year, at most, are available through these sources. Even exploratory calculations in quantum chromodynamics require several CRAY CPU hours. The acquisition of a supercomputer at the University of Illinois is, therefore, essential to the continuance of this research program.

The types of research accessible to computer simulation by field theorists is enormous. The Illinois group, in addition to studying quantum chromodynamics from the elementary particle perspective, has completed applications to heavy-ion collisions, neutron stars and cosmology.[6] Quantum chromodynamics has been simulated at finite temperatures and in environments rich in baryon number.[7] Quark confinement and chiral symmetry breaking have been studied systematically in each case. More theoretical topics such as non-perturbative calculations in supersymmetric field theories and the role of topological excitations in gauge theories are in the planning stages.

With our experience on CRAY level machines and medium scale parallel processors, we would use a local supercomputer facility effectively from the date of delivery. We have in hand several projects which would require many supercomputer hours. This includes systematic work on supersymmetric models and the inclusion of light dynamical quarks into accurate simulation procedures. Both of these topics have the potential of breaking new ground in the field.

At this time our theory group is developing, in collaboration with the Illinois Materials Research Laboratory, a VAXNET/FPS-164 system for computer simulations. The medium size FPS-164 array processor is proving quite productive. For vector codes it achieves a good fraction (1/3-1/2) of its ideal speed of 12 megaflops. Typically, these codes run ten times faster on the CRAY-1A of Los Alamos and, presumably, would run faster yet on more recently developed supercomputers. Therefore, we foresee a very productive interplay between our local, medium-size FPS-164 facility and the supercomputer. Small and medium size jobs could run effectively on the FPS-164 and program development and vectorization could be done there. Thorough, large scale simulations could then be run much more efficiently on the supercomputer. In addition, the superb software, graphics, curve fitting, and data analysis packages on the supercomputer such as the CRAY X-MP have no match on the smaller VAXNET/FPS-164 system. In our work on the CRAY-1A at Los Alamos such software has been extremely useful.

We envisage a network linking the supercomputer to the VAXNET/FPS-164 for optimal usage of both excellent facilities. In addition to increasing our research productivity, this network will aid physics students in learning the art of computer simulation and high energy field theory simultaneously. Our facilities will provide students with opportunities that have not been available to other research-oriented universities in the country. We have graduated several undergraduate and graduate students in the last few years with similar, but lesser backgrounds, and they are proceeding toward excellent careers at first-rate institutions.

References

(1) For recent reviews see J. Kogut, "An Introduction to Lattice Gauge Theory and Spin Systems," Rev. Mod. Phys. *51,* 659 (1979) and "A Review of the Lattice Gauge Theory Approach to Quantum Chromodynamics," Rev. Mod. Phys., *55,* 775 (1983).

(2) K. G. Wilson, "Confinement of Quarks," Phys. Rev. *D10,* 2445 1974).

(3) M. Creutz, "Asymptotic Freedom Scales," Phys. Rev. Lett. *45,* 313 (1980): "Monte Carlo Study of Quantized SU(2) Gauge Theory," Phys. Rev. *D21,* 2308 (1980).

(4) J. Kogut, M. Stone, H. W. Wyld, Jr., J. Shigemitzu, S. H. Shenker, and D. K. Sinclair, "The Scales of Chiral Symmetry Breaking in Quantum Chromodynamics," Phys. Rev. Lett. *48,* 1140 (1982) and with W. R. Gibbs, "Deconfinement and Chiral Symmetry Restoration at Finite Temperatures in SU(2) and SU(3) Gauge Theories," Phys. Rev. Letter. *50,* 393 (1983).

(5) J. Stack, "The Heavy Quark Potential in SU(2) Gauge Theory," Phys. Rev. *D27,* 412 (1983).

(6) J. Kogut, H. Matsuoka, M. Stone, H. W. Wyld, J. Shigemitsu, S. H. Shenker, and D. K. Sinclair, "Quark and Gluon Latent Heats at the Deconfinement Phase Transition in SU(3) Gauge Theory," Phys. Rev. Lett. *51*, 869(1983).

(7) J. Kogut, H. Matsuoka, M. Stone, H. W. Wyld, J. Shigemitsu, S. H. Shenker, and D. K. Sinclair, "Chiral Symmetry Restoration in Baryon Rich Environments," ILL-(TH)-83-10, April 1983.

A partial list of publications by members of the high energy theory group which have relied on large scale computer simulations are, in addition to references 4-7 on the previous page:

(8) J. Kogut, M. Stone, and M. Snow. Mean Field and Monte Carlo Studies of SU(N) Chiral Models in

Three Dimensions. Nucl. Phys. *B200,* 211 (1981).

(9) J. Kogut, M. Stone, and M. Snow. Computer Simulations of SU(N) v SU(N) Spin Systems in Two Dimensions. Phys. Rev. Lett. *47,* 1767 (1981).

(10) J. Kogut, C. J. Hamer, D. P. Crewther, and M. M. Mazolini. The Massive Schwinger Model on a Lattice: Background Field, Chiral Symmetry and the String Tension. Nucl. Phys. *B208* 413 (1982).

(11) J. Kogut, M. Stone, and M. Snow. SU(N) v SU(N) Spin Systems in Two Dimensions: Crossover, Variant Actions and Finite Size Scaling. Nucl. Phys. *B215,* 45 (1983).

(12) J. Kogut, M. Stone, H. W. Wyld, J. Shigemitzu, S. H. Shenkar, and D. K. Sinclair. Studies of Chiral Symmetry Breaking in SU(2) Gauge Theory. Ohio State University preprint, May 1983.

(13) J. Kogut, J. Bartholomew, J. Sloan, M. Stone, and S. H. Shenker. Chiral Symmetry Breaking in Lattice Electrodynamics. Illinois preprint, Sept. 1983.

(14) J. Stack, G. Jongeward, and C. Jayaprakash. Monte Carlo Calculations on Z(2) Gauge-Higgs Theories. Phys. Rev. *D21,* 3360 (1980).

(15) J. Stack. The Heavy Quark Potential in SU(3) Gauge Theory. Institute for Theoretical Physics preprint, June 1983.

(16) H. W. Wyld, H. H. Roomany, and L. E. Holloway. New Method for the Hamiltonian Formulation of Lattice Spin Systems. Phys. Rev. *D21,* 1557 (1980).

(17) H. W. Wyld and H. H. Roomany. Finite-Lattice Approach to the 0(2) and 0(3) Models in 1 + 1 Dimensions and the (2 + 1)-Dimensional Ising Model. Phys. Rev. *D21,* 3341 (1980).

(18) H. W. Wyld and H. H. Roomany. Finite Lattice Hamiltonian Results for the Phase Structure of the Z(Q) Models and the Q State Potts Model. Phys. Rev. *B23,* 1357 (1981).

MANY-BODY APPROACH TO THE ELECTRONIC STRUCTURE OF SOLIDS

A. Barry Kunz - Professor

Department of Physics & Materials Research Laboratory

The theory of electronic structure of solids has developed along two parallel lines. The first of these, based upon the density functional formalism and the Hohenberg-Kohn theorem, has been recently quite successful in delineating the ground state properties of extended systems, but has been much less successful in predicting the excitation properties of such systems. The second method is to use the techniques of Many-Body theory (principally Many-Body-Perturbation-Theory or Green's Function methods) to construct theories of the electrically excited states of solids and large molecules. These approaches have been substantially hampered by their inherent computer intensive nature. Access to adequate large memory high speed computers has not been available to enough scientists to have permitted these techniques to evolve into generally useful algorithms or to permit many systems to be explored. In general such methods rely extensively on matrix methods and are thus ideal problems for solution on vector computers.

The specific applications envisioned by the group associated with Kunz is to continue to construct methods based upon degenerate state perturbation theory to permit the study of localization of quasiparticles in periodic systems. Specific examples are the localization of hole states in the core bands of all types of solids and the detailed nature of the modification of the surrounding electronic cloud. In addition the attraction of this local core hole and its distorted electronic surroundings for the electron generated during the creation of the hole state will be studied. That is, the entire range of core-exciton phenomena will be investigated. This study is to encompass insulators as well as metals. Substantial initial progress has been made in the study of core holes and excitons in insulators. Spectral line positions and multiplet splittings, accurate to better than 0.1 eV have been obtained for several systems. This is the first time that first principles determination of the multiplet structure in a core exciton has been made. Related studies into the spectrum of impurities in solids are planned as well.

A related but somewhat different study concerns the nature of valence excitons and related excitonic resonances in solids. In these cases the hole state is not localized in space but migrates in the crystal with an electron forming a Bloch like exciton. Such phenomena are well established in insulators and semiconductors and are recently postulated to exist in polyvalent metals as well. Semi-empirical theories cope well with such systems as semiconductors, but are less well established in the insulators where multiplet effects are possibly dominant. We propose to conduct such studies.

Kunz has had in excess of twenty years experience in performing large scale computations. He was one of the original scientists to perform studies on the then revolutionary CDC 6600 in 1965. More recently he has been limited to access to more conventional computers such as the VAX or the Cyber 175 on campus. Recently he has had much experience in programming and running programs on an FPS 164 attached processor. This processor is in many respects a vector machine and in that type of operation performs about two times faster than the Cyber 175. The preliminary results referred to were obtained on the FPS 164. It is not possible to make a definitive estimate of supercomputer time needed but a ball park estimate would be 100 hours per year. With little modification of existing codes, problems in localization and excitons could be initiated on a supercomputer at full vector speeds as soon as it becomes available.

References Reflecting Large Scale Computation

L. A. Grunes, R. D. Leapman, C. N. Wilker, R. Hoffmann, and A. B. Kunz, Oxygen K near edge fine structure: An electron-energy-loss investigation with comparisons to new theory for selected 3d transition-metal oxides, Phys. Rev. B25, 7157-7173 (1982).

A. Y. S. Kung, A. B. Kunz, and J. M. Vail, Unrestricted-Hartree-Fock cluster analysis of F and FA centers in some alkali halides. Phys. Rev. B26, 3352-3360 (1982).

A. B. Kunz, Study of the electronic structure of twelve alkali halide crystals. Phys. Rev. B26, 2056-2069 (1982).

A. B. Kunz, Electronic structure of AgF, AgCl and AgBr. Phys. Rev. B26, 2070- 2075 (1982).

A. B. Kunz and J. T. Waber, A theoretical study of the binding of positrons to gaseous molecules in positron annihilation, eds. P. G. Coleman, S. C. Sharma, and L. M. Diana, (North Holland), 113-115 (1982).

A. B. Kunz and C. P. Flynn, A new configuration interaction method for excitons and interband processes applied to LiF, J. Phys. C16, 1659-1663 (1983).

A. B. Kunz and C. P. Flynn, Excitonic effects in the interband spectra of metals, Phys. Rev. Lett. 50, 1524-1527 (1983).

Recent Participation in Computer Panels

A. Barry Kunz

(1) June 1981 -- The then National Resource for Computational Chemistry had a final conference terminating its program at Los Alamos entitled "Effective Potentials for Quantum Chemistry," at which I was an invited speaker and presented two talks.

(2) 6-12 March 1983 -- The Sanibel Symposium on Quantum Chemistry received funding from the National Science Foundation and from the Physics Directorate of the Office of Naval Research. As part of this symposium a subsection on "Computers in Quantum Chemistry and Condensed Matter Theory" was included. This covered the range of micro's, super-mini's (VAX etc.), array processors (chiefly FPS-164), main frames (mostly IBM 30nm or Cybers) and supercomputers (chiefly CRAY 1's). My participation in this was two-fold. I served on the advisory committee which organized the symposium and I also served on a panel which investigated future directions for computing in this area. My report has been accepted for publication in the conference proceedings and a report from this subsymposium is in preparation for issue to the funding agencies.

SIMULATION OF DISORDERED SOLIDS

William L. McMillan - Professor

Department of Physics

Development of analytic theory for many disordered systems - spin-glasses, random ferro-magnets, glasses and amorphous conductors - remains a challenging problem in solid state physics. Numerical simulation, using Monte Carlo or other appropriate simulation tools, can be useful both in comparing models to experiment and in guiding one to the right analytic approximations.

Electrons in amorphous metals or semiconductors see a random potential as well as the coulomb interaction with other electrons. The outlines of an analytic theory have been sketched[1,2]; and simulation can be an important tool in developing more completed realistic theoretical approaches. The most efficient way to find the properties of electrons in a random potential is through numerical integration of the time-dependent Schrodinger equation. One finds the Green's function which can be used to calculate physical properties such as conductivity or the density of states. For non-interacting electrons one can study realistic Hamiltonians for, say, binary alloys of transition metals. The most important interaction effects can be included with the Hartree-Fock approximation. One can study the question of multiplicity of ground states and of non-equilibrium effects due to relaxation between ground states.

Extensive Monte Carlo simulations (on the Urbana Monte Carlo computer) of two-dimensional spin-glass models[3] have been able to characterize the equilibrium and dynamic behavior of the models. System equilibration times become very long at low temperature and very extensive computer runs are required. Based on these simulations, the beginnings of an analytic theory of spin-glasses has been proposed.[4] Three-dimensional Monte Carlo simulations and Monte Carlo renormalization group methods would also be very helpful in the development of a believable analytic theory.

Transfer matrix simulations performed on an FPS-164 attached processor have proven very effective in studying the low temperature equilibrium properties of the two-dimensional Ising spin glass models. The computations are far more time-consuming in three dimensions but may be feasible on a supercomputer. The three dimensional Ising spin-glass model is currently the most important unsolved model and the combination of Monte Carlo and transfer matrix methods may be sufficient to characterize the model. I believe that long runs (several hundred hours may be necessary) during the first year of Illinois supercomputer operation may yield important results on this difficult problem. Such simulations, if successful, could suggest new analytic methods and a qualitatively improved understanding of spin glasses.

The computations proposed above are easily vectorized to run effectively on a supercomputer. Further, it is standard procedure to code the dominant routines in machine language to take full advantage of the hardware. I believe that the simulations are important enough to the development of the theory of the amorphous solid state that the investment in computer time is fully justified.

References

(1) W. L. McMillan, "Scaling Theory of the Metal-Insulator Transition in Amorphous Materials," Phys. Rev. B *24*, 2739 (1981).

(2) E. Fradkin and M. Ma, "Localization and Interactions in a Disordered Electron Gas," Illinois preprint, March 1983.

(3) W. L. McMillan, to be published.

(4) W. L. McMillan, to be published.

RESEARCH IN MANY BODY SYSTEMS

Vijay Pandharipande - Professor

Department of Physics

There were significant developments in the microscopic many-body theory in the seventies. The Green's function Monte Carlo method[1] to calculate, in an exact fashion, the ground state properties of many-body systems became a "standard tool." New and more realistic variational wavefunctions were developed[2] for condensed quantum systems such as solid and liquid ^{4}He and ^{3}He, nuclear and neutron-star matter etc. Studies of finite or other inhomogeneous systems are now possible, and, within the framework of the correlated-basis-functions theory[3], we can also study elementary excitations and finite temperature properties over a wide temperature range. There now appears to be a definite possibility to go far beyond the Landau's low temperature region with a microscopic theory.

The Monte Carlo calculations with realistic wavefunctions are very computer limited. In a recent study[4] of droplets of ^{4}He liquid, it took about 200 hours on the IBM 370/195 at Argonne National Laboratory to execute variational calculations of droplets containing up to 724 atoms, and about 200 hours on the Cyber 205 at Bochum were used for Green's function calculations of droplets having up to 112 atoms. Estimates of computer requirements for similar study of Fermi liquid drops are much higher.

Availability of a supercomputing facility at the Urbana-Champaign campus will open up many new areas in microscopic many-body theory. We list a few of them, which are directly related to our present program with brief comments wherever necessary.

(1) Oscillations of quantum (Bose) liquid drops and their relation to bulk surface and volume excitations.
(2) Behavior of impurities such as hydrogen and ^{3}He on surface of ^{4}He liquid and eventually on metal surfaces.
(3) Drops and surfaces of Fermi liquids.
(4) Fermion Green's function Monte Carlo. The ground state energies obtained with the best variational wavefunctions are just a few percent above the presumably exact energies for Bose systems. Thus, by starting from the best available Fermion wavefunctions it may be possible to obtain convergent Green's function Monte Carlo estimates before the Bose noise becomes too great.
(5) Variational Monte Carlo calculations of nuclei: Spin and isospin dependent correlations and interactions have made these calculations very difficult. With realistic Hamiltonians only nuclei with 3 and 4 nucleons have been simulated so far. Our knowledge of three nucleon interaction will be much richer when we can calculate the properties of larger nuclei for which much experimental data exists.
(6) Energies and decay of nuclear giant oscillations.
(7) Elementary excitations and finite temperature properties of liquid ^{3}He, ^{4}He and nuclear matter.
(8) Calculations of collisions between bound states of few-body systems. Rich experimental data exists on reactions between light nuclei. It may be of interest to study hadron-hadron collisions where a hadron is represented by a few quark states.
(9) Collisions between relativistic heavy ions.

We are currently collaborating in a study of the problems (1) and (3) listed above, using the computer facilities at Argonne National Laboratory (IBM 370/195), and at Ruhr University at Bochum (Cyber 205) (W. Germany). Dr. Kevin Schmidt, with whom we collaborate often, is studying problem (5) at Los Alamos (CRAY-1). We will attempt to use the FPS array processor in the Materials Research Laboratory at the University of Illinois Urbana for problem (2).

The present computer resources available to us are not sufficient to study problems (3) and (5) in a realistic fashion. Drops of liquid ^{3}He with less than 40 particles are not bound; however, we cannot work with this many particles on the IBM 370/195. Hence we are studying a model problem designed such that only 8 particles form bound states. We believe that about 200 hours on a supercomputer are needed to study drops and surface properties of liquid ^{3}He. Another 200 hours is needed to study 8-body nuclei with

realistic Hamiltonians. Problems (4) and (8) will be studied, in the context of realistic systems, after the initial investigations of (3) and (5). Access to a supercomputer on campus will give us the raw computing power which should open new pathways for developments, both numerical and analytic, in both the few-nucleon and liquid ^{3}He problems. Further developments beyond that are possible and are equally, or even more, exciting. Investigations in topics (8) and (9) will overlap with the work of the high energy theory group (J. Kogut) and we anticipate additional collaborative efforts there. The construction of heavy-ion colliders and the experimental study of nuclear matter in extreme environments will further stimulate our work in topic (9). It is becoming quite clear to many researchers in our field that supercomputing power has the potential to dramatically advance our understanding in a host of interesting, timely problems concerning many body systems.

References

(1) M. H. Kalos, M. A. Lee, P. A. Whitlock, and G. V. Chester, "Modern Potentials and the Properties of Condensed ^{4}He," Phys. Rev. *B24,* 115 (1981). M. A. Lee, K. E. Schmidt, M. H. Kalos, and G. V. Chester, "Green's Function Monte Carlo Method for Liquid ^{3}He," Phys. Rev. Lett. *46,* 728 (1981). J. G. Zabolitzsky, K. E. Schmidt, and M. H. Kalos, "Exact Ground States of Few-Body Nuclei With and Without Three-Body Forces," Phys. Rev. *C25,* 1111 (1982).

(2) Q. N. Usmani, S. Fantoni, and V. R. Pandharipande, "Three-Body Correlations in Liquid ^{4}He+," Phys. Rev. *B26,* 6123 (1982). K. E. Schmidt, M. A. Lee, M. H. Kalos, and G. V. Chester, "Structure of the Ground State of a Fermion Fluid," Phys. Rev. Lett. *47,* 807 (1981). J. Carlson, V. R. Pandharipande, and R. B. Wiringa, "Variational Calculations of Resonant States in ^{4}He," Submitted to Nucl. Phys. for publication (1983).

(3) S. Fantoni, V. R. Pandharipande, and K. E. Schmidt, "Single-Particle Spectrum and Specific Heat of Liquid ^{3}He," Phys. Rev. Lett. *48,* 878 (1982). S. Fantoni, B. L. Friman, and V. R. Pandharipande, "Correlated Basis Theory of Nucleon Optical Potential in Nuclear Matter," Nucl. Phys. *A399,* 51 (1983).

(4) V. R. Pandharipande, J. G. Zabolitzsky, S. C. Pieper, R. B. Wiringa, and U. Helmbrecht, "Calculations of ground state properties of liquid ^{4}He droplets", Phys. Rev. Lett. *50,* 1676 (1983).

LARGE MOLECULE AB INITIO ELECTRONIC STRUCTURE CALCULATIONS

Clifford E. Dykstra - Associate Professor

Department of Chemistry

Ab initio calculations of the electronic structure of even a simple molecule is an elaborate process. Millions of intermediate quantities are evaluated and processed. Nonetheless, the electronic structure of many molecules can be predicted quantitatively, challenging experimental measurements in very many instances. The difficulty that still persists, though, is that the calculational costs have a much worse than linear dependence on the number of electrons. A mere 40-electron molecule is "big" by the standards of the most reliable treatments.

The most subtle feature in electronic structure is the instantaneous rather than averaged interactions of electrons that give rise to correlation of their motions. We have developed pair correlation approached[1-4] that make possible accurate calculations of electron distributions. These approaches all use a pair coefficient matrix representation of the wavefunction in terms of original atomic orbitals. Associated matrix operators are used to solve for the wavefunction. This eliminates certain redundancies in conventional methods because all operations are carried out collectively for sets of correlating electron configurations. Thus, it is immediately suited to vector and array processors. *

In addition to developing new techniques for treating electron correlation, we are also interested in methods for electron repulsion integrals and for self-consistent field (SCF) wavefunctions that can take advantage of supercomputers. We have developed a direct SCF method[5] that overcomes the practical limit on the number of electrons by restructuring nearly all operations into simple vector dot products. Lacking a supercomputer, however, we are unable to do more than simulate certain features of its performance.

Currently, we are working on a variation in the Rys polynomial exact quadrature method[6] for evaluating integrals. We are developing a program that performs certain operations collectively for blocks of intermediate values. It ends up with integrals arranged in operator form as needed for both our direct SCF and operator correlation methods. Again, the availability of a supercomputer would enable us to look at larger sized problems.

There are a number of very different large molecule chemical studies that could be undertaken using our methods on a supercomputer. Perhaps the most interesting of these studies and the one that would receive immediate attention is cluster magnesium chemistry. We have recently reported calculations [7] demonstrating strong magnesium-magnesium bonding in what we have termed cluster Grignards. These are viable chemical species that may have already been seen in matrix codeposition experiments. [8] Since our work on the Mg^4 cluster [9] that showed a remarkable hybridization and unexpected chemical bonding arising from electron correlation effects, we have felt that magnesium clusters may be important reaction sites. Dimagnesium molecules we have studied so far support this, and with a supercomputer we would expect to study the following.

(1) Stabilities of RMg_3X, RMg_4X and $(RMg_2X)_2$

(2) The reaction path and barrier for $(RMg_2X)_2$ to RMg_2X and then to RMgX.

(3) The abstraction of magnesium and magnesium clusters from a larger cluster upon chemical attack.

New computing architecture is having a very strong impact on all areas in molecular electronic structure theory. The use of array processors and supercomputers is being reviewed and assessed and continues to look very promising.** In fact, we expect to utilize about 100 hours of supercomputer time on the proposed supercomputer during its first year on campus.

* Currently, a joint NSF proposal with R. J. Kirkpatrick is pending. It will allow us to acquire a Floating Point Systems Attached Arithmetic Processor, Model 164. This will be used to study NMR chemical shifts in silicates.

** For example, a NATO Advanced Research Workshop is being held in September 1983 in Colorado Springs on "Vectorization of Advanced Methods for Molecular Electronic Structure. An assessment of State-of-the-Art Electron Correlation Theories and Unifying Features Suited to Vectorized Computation". [Organizing Committee: R. Ahlrichs, W. Meyer and C. E. Dykstra, Chairman]

References

(1) C. E. Dykstra, H. F. Schaefer and W. Meyer, J. Chem. Phys. *65,* 2740 (1976).

(2) C. E. Dykstra, R. A. Chiles and M. D. Garrett, J. Comp. Chem. *2,* 266 (1981).

(3) R. A. Chiles and C. E. Dykstra, J. Chem. Phys. *74*, 4544 (1980).

(4) P. G. Jasien and C. E. Dykstra, J. Chem. Phys. *76*, 4564 (1982).

(5) M. A. Benzel and C. E. Dykstra, J. Comput. Chem. *3,* 260 (1982).

(6) H. F. King and M. Dupuis, J. Comput. Phys. *21,* 144 (1976): M. Dupuis, J. Rys and H. F. King, J. Chem. Phys. *65,* 111 (1976); J. Rys, M. D. Dupuis and H. F. King, J. Comput. Chem. *4,* 000 (1983).

(7) P. G. Jasien and C. E. Dykstra, J. Am. Chem. Soc. *105,* 2089 (1983).

(8) Y. Tanaka, S. C. Davis and K. J. Klabunde, J. Am. Chem. Soc. *104*, 1013 (1982).

(9) R. A. Chiles, C. E. Dykstra and K. D. Jordan, J. Chem. Phys. *75*, 1044 (1981).

MONTE CARLO STUDIES OF CHEMICAL QUANTUM DYNAMICS IN CONDENSED PHASES

Peter G. Wolynes - Professor

Department of Chemistry

The computational research in my group centers on the use of quantum statistical mechanics to understand the dynamics of chemical reactions in liquids, solids and amorphous phases. Our goal is to close the gap between the electronic structure and the configurational dynamics aspect of the problem. This had led us to the use of path integral Monte Carlo methods like those used in elementary particle physics.

In the past, most problems in the chemical physics of condensed phases were treated as if they had two separate aspects. The first of these is understanding of the electronic structure of the interacting species. This information is summarized in a potential energy surface for the nuclei. After some semblance of this understanding is achieved there remains the statistical mechanical problem of discovering how the motion of the interacting molecules leads to the observed chemical phenomena. The separation of the problem into two parts relies on the Born-Oppenheimer approximation. The basis of this approximation is that the timescale of electronic motion is generally shorter than the timescale of the motion of the nuclei in the molecules because of the considerable disparity in the masses of the particles. Although this standard approximation in theoretical chemistry is often quite good, it obscures the intimate connections between the many body physics of the condensed phase and the delicate few body phenomena of the electronic structure of the constituent molecules.

When electrons are not well-localized or when their degree of localization changes with displacement of the nuclei, the Born-Oppenheimer potential cannot be easily decomposed into few body contributions. In chemical physics there are many situations in which the electrons in a molecule are not well localized. The physically simplest example is the solvated electron.[1] This species, very important in radiation chemistry, consists of an electron trapped in a potential well caused both by the distortion of nearby solvent molecules in the cage and by polarization induced in distant solvent molecules. Other examples can be found among conjugated molecules such as dyes. Here there are significant solvatochromic shifts of the energy levels of the π -electron system when the molecules are immersed in a condensed phase. There is usually less localization in excited states than in ground states. Rydberg states[2] and molecular exciton states[3] are often fairly delocalized in condensed phase systems.

More ubiquitous than these systems which have delocalized electronic states for the most probable molecular configurations are systems which are delocalized in the transition state configurations for chemical reactions. When the electronic structure is very different in reactants and products the transition state whose free energy determines the rate of reaction often has a delocalized electronic structure. In an electron transfer reaction the transition occurs when the solvent is in a nonequalibrium configuration for which the energy of reactant and product would be equal if electron tunneling were neglected.[4] Thus, for this transition state configuration the transferred electron is delocalized between two centers. The solvent easily changes the balance between the localized reactant state and the delocalized transition state and is therefore an important contributor to the activation energy. When only neutral species are involved but chemical bonds are broken and made during the reaction there is also considerable delocalization in the transition state. In the dynamics of these chemical reactions one also can face the breakdown of the Born-Oppenheimer approximation.[5] The delocalization in the transition state arises from a near degeneracy of electronic states. This near-degeneracy means that the timescale of electronic motion is considerably longer than usual. In many cases, then, the separation of timescales between electronic and nuclear motion fails. When this occurs both the nuclei and the electrons must be treated quantum mechanically.

In surveying these problems in condensed matter chemical physics we see that the common theme is that of describing a localized state strongly interacting with its environment and of describing the changes in the degree of localization. It seems appropriate, then, to formulate the problem in a way that allows full attention to be paid to the local dynamics of the system and to pay less attention to the details of the dynamics of the environment. A similar situation occurs in the study of the classical dynamics of chemical phenomena. [6] An appropriate approach here is to use a stochastic or Langevin dynamics scheme to focus on the relevant degrees of freedom. Classically when "irrelevant" degrees of freedom are removed from explicit

consideration their effects remain as potentials of mean force that summarize their static effects and as frictional and random forces that summarize their dynamic effects. A parallel development is possible in quantum mechanics if the path integral formation of quantum mechanics is used.[7] In quantum mechanics the effects of the environment are summarized in an influence functional.[8]

The remaining statistical mechanical problems involve the calculation via Monte Carlo methods of various quantum mechanical and thermal averages using the path integral.

So far we have investigated some simple caricatures of the real chemical physics problems using two-level systems coupled to a many oscillator environment. This is a reasonable model for the transition states of electron transfer reactions as well as for Josephson junctions. We have made many technical advances in this work. Foremost among these have been convenient and accurate path integral quadratures, more accurate than those used elsewhere.[9] Furthermore, we have developed methods for performing path integrations for real time dynamics.[10] This is necessary for the calculation of spectra and chemical reaction rates. The difficulty here is that for real time dynamics the path integral expressions involve nonpositive weights. We have learned how to deal with these in a brute force manner and currently are developing methods of importance sampling to improve the accuracy.

The models we have studied so far involve only a few degrees of freedom coupled to a many body environment. New problems arise if these degrees of freedom refer to indistinguishable particles, an essential when dealing with problems of a covalent electron pair bounding phenomena. The obvious question in the present context is how chemical bonding is affected by the condensed phase environment. An important qualitative feature is that the environment changes the electron correlation effects. In addition to the short range electron-electron repulsion there is a long range attraction. One electron transiently polarizes its environment and the other electrons are attracted to the potential well. Here it is worth remarking on the similarity to the physics of quark confinement.

In the path sums for indistinguishable particles one must include paths in which the identities of the particles have been interchanged. This again leads to nonpositive weights for the low temperature fermion problem. When there are not too many electrons explicitly considered in the calculation there is an alternative approach since there is nothing sacrosanct about using the position space representation for quantum paths. If other intermediate states are used in the path sum much of the cancellation can be circumvented. A useful choice is to use fully antisymmetric intermediate states built up out of Slater determinants of Hartree-Fock orbitals. We have investigated the possible use of Fock space states in few fermion Monte Carlo for isolated molecules. We are further developing these methods for molecules in solvents. Our goal here is to develop effective potentials for molecules in solvents that will allow us to study their dissociation. This will be a useful step in current studies of proton transfer reactions in water and other solvents.

We believe these new simulation techniques are an important step to understanding chemistry in complex many body systems. Most of our work to date has been developmental. In this stage we use the VAX 11/780 at the rate of about 2000 hours per year. We are presently beginning to vectorize our calculations for a Floating Point Systems array processor. Therefore, we would be set to easily use 300 hours of supercomputer time the first year it is on campus and even more once we are past the developmental stage.

References

(1) L. Kevan and B. Webster: 1976, Electron-Solvent and Anion-Solvent Interactions, Elsevier.

(2) J. Jortner and C. A. Coulson: 1961, Mol. Phys., *4*, pp. 451-464.

(3) S. A. Rice: 1968, Acc. Chem Res., *1*, pp. 81-96.

(4) R. A. Marcus: 1956, J. Chem. Phys., *24*, pp. 979-989.

(5) J. Ulstrup: 1979, Charge Transfer Processes in Condensed Media, (Springer-Verlag) pp. 79-94.

(6) S. A. Adelman: 1980, Adv. Chem. Phys., *44*, pp. 143-254.

(7) R. P. Feynman and A. R. Hibbs: 1965, Quantum Mechanics and Path Integrals, McGraw-Hill, New York, p. 365.

(8) R. P. Feynman and F. L. Vernon: 1963, Ann. Phys. *24*, pp. 118-173.

(9) K.S. Schweizer, R. M. Stratt, D. Chandler and P. G. Wolynes: 1981, J. Chem. Phys., *75*, pp. 1347-1364.

(10) P. G. Wolynes: 1984, Monte Carlo Methods for Quantum Problems, NATO Workshop proceedings, M. Kalos, editor.

Related publications on Path Integral Methods for Chemical Physics Problems by the Illinois Group.

(11) D. Chandler and P. G. Wolynes: 1981, J. Chem. Phys., *74*, pp. 2078-2095.

(12) D. Chandler, K. S. Schweizer and P. G. Wolynes: 1982, Phys. Rev. Lett., *49*, pp. 1100-1103.

(13) P. G. Wolynes: 1981, Phys. Rev. Lett., *47*, pp. 968-971.

GLOBAL ATMOSPHERIC CIRCULATION AND CUMULUS PARAMETERIZATION

Yoshi Ogura - Professor and Head
Su-Tzai Soong - Associate Professor

Department of Atmospheric Sciences

It has long been recognized that the release of latent heat in deep cumulus convection plays a major role in the energetics of the global atmospheric circulation. Cumulus convection and the associated latent heat release is also an important energy source on a much smaller scale. Satellite observations have shown that clouds are commonly organized into "clusters" with horizontal scales of several hundred kilometers. In the intense, but less frequently occurring, tropical cyclone it appears that the organized heating of deep convection plays a major role in the transformation from an open wave to a closed vortex and in its subsequent development. Besides emphasizing the role of deep convection, recent studies of the tropical heat and moisture budgets over areas of several hundred to a thousand kilometers have made it clear that shallower cumulus clouds play an important role in transporting moisture upward into the lower and middle troposphere, thereby counteracting the drying effects of the deep clouds.

Since the horizontal scale of individual cumulus clouds is of the order of several kilometers it is impractical to resolve them in any numerical model of the larger scale circulation where a typical horizontal grid spacing is a few hundred kilometers. Instead, the collective influence of clouds within a larger area must be formulated, or parameterized, in terms of the large-scale environmental variables. Therefore, the goal in cumulus parameterization is to predict the changes in the large-scale variables due to cumulus convection from the known large-scale variables. It is by no means obvious that this goal is always attainable. However, the organization of individual clouds into clusters indicates that cumulus convection is not a random process; instead, it may be controlled by the larger-scale dynamical and thermodynamical processes. Moreover, the fact that the time and space scales of individual cumulus clouds are distinctly smaller than those of the large-scale disturbance in which they form has encouraged scientists in their attempts to solve the problem of cumulus parameterization.

Ogura and Soong are developing a cumulus parameterization scheme, possibly through modification of existing schemes, for the purpose of improving cloud and precipitation forecasting on the global scale. To achieve this objective, the following three steps are being taken.

(1) Evaluation of the physical basis of the existing cumulus parameterization schemes. This step has been completed.

(2) Tests of the parameterization schemes using a fine-grid model for organized convective systems. In a separate project, Soong and Ogura (1980) developed a model which they call a cumulus ensemble model in both two and three dimensions. As far as physical processes represented in the model are concerned, the cumulus ensemble model is essentially similar to the non-hydrostatic moist cloud model described in Soong and Ogura (1973). However, the model has been developed to investigate statistical properties of a group of cumulus clouds under a prescribed large-scale forcing, rather than investigating the structure and evolution of an isolated storm. Accordingly, this model permits several clouds of various sizes to develop simultaneously in the model domain. The model was applied by Soong and Tao (1980) and Tao (1982) to the intense tropical cloud band which developed during the GARP Atlantic Tropical Experiment. The model-derived cloud heating and drying effects were found to agree well with the observations. Moreover, some statistical properties of the model clouds were consistent with those measured by air-borne instruments. Presently cloud properties predicted implicitly or explicitly by the existing cumulus cloud parameterization schemes are being compared with those derived from the cumulus ensemble model.

(3) Tests of the parameterization scheme in a global circulation model. Since a good parameterization needs to be valid for vastly different atmospheric conditions, the final step of this research project is to apply one or two promising schemes to a global circulation model (GCM). The GCM we use for this purpose is basically the same as that developed and being used operationally by the National

Meteorological Center. In essence, this is a spectral model, with a rhomboidal 12-layer, 30 zonal wave. We expect to start running this GCM on the CRAY-1 at the National Center for Atmospheric Research shortly.

Once a good cumulus parameterization is developed, it will be applied not only to a GCM, but also to a limited-area fine-mesh model (LFM) nested in the GCM. The lateral boundary conditions for the LFM will be given from the output of the GCM in an interactive manner. The objective here is to improve the prediction of local precipitation. Our immediate interest is in the structure and temporal evolution of cold fronts, since much of the significant weather in mid-latitudes is associated with the passage of cold fronts. Recently Ogura and Portis (1982) analyzed the data gathered for a well defined cold front event from a special observation program in 1979 known as SESAME. The results indicate that the theory proposed by Hoskins and Bretherton (1972) is able to predict the gross frontogenesis processes qualitatively; however, it fails to predict the development of a narrow band of strong horizontal convergence along the cold front. The presence of this narrow convergence band is essential for triggering and sustaining heavy precipitation along the front. The acquisition of a supercomputer will permit us to increase the vertical and horizontal resolutions of the LFM, to incorporate more physical processes into the LFM and to study precipitation processes in different synoptic weather situations. We estimate that we will use about 100 hours during the first year the supercomputer is available.

References

Hoskins, B. J., and F. P. Bretherton, 1972: Atmospheric frontogenesis models: Mathematical formulation and solution. J. Atmos. Sci., *29*, 11-37.

Ogura, Y., and D. Portis, 1982: Structure of the cold front observed in SESAME-AVE III and its comparison with the Hoskins-Bretherton frontogenesis model. J. Atmos. Sci., *39*, 2773-2792.

Soong, S. T., and W. K. Tao, 1980: Response of deep tropical cumulus clouds to mesoscale processes. J. Atmos. Sci., *37*, 2016-2034.

Soong, S. T., and Y. Ogura, 1980: Response of trade-wind cumuli to large-scale processes. J. Atmos. Sci., *37*, 2035-2050.

Soong, S. T., and Y. Ogura, 1973: A comparison between axi-symmetric and slab-symmetric cumulus cloud models. J. Atmos. Sci., *30*, 879-893.

Tao, W. K., 1982: A numerical study of the structure and vertical transport properties of a tropical convective system. Ph.D. Dissertation Department of Atmospheric Sciences, University of Illinois, 233 pp.

DYNAMICS OF SEA ICE

John Walsh - Associate Professor

Department of Atmospheric Sciences

Sea ice has long been regarded as a key component of the global climate system. However, large-scale interactions between sea ice, the atmosphere and the ocean are exceedingly complex. First, the ice is constantly moving in response to winds and ocean currents. These driving forces can cause the ice to advance well beyond the line of thermal equilibrium. Second, the heat balance and the wind and currents themselves are affected by the presence of ice. In addition to a variety of small-scale interactions, ice influences the atmosphere and ocean on a large scale by cutting off the fluxes of heat and moisture from the ocean to the atmosphere, by reflecting or absorbing shortwave radiation that would otherwise warm the ocean, by producing dense salty water during freezing, and by producing light, fresh water during melting.

Prior to the availability of recent generations of high-speed computers, the only studies of large-scale ice-atmosphere interactions were empirical analyses of observational data. The empirical analyses were limited to regions for which ice data had been archived, and these analyses were restricted to routinely observed variables (atmospheric pressure and temperature, ice extent); other climatically relevant variables (ice thickness, vertical heat fluxes, horizontal heat and mass transports) cannot be determined observationally. Empirical studies also suffer from the limitations that atmospheric wind and temperature anomaly fields are not independent, thereby precluding quantitative evaluations of dynamic and thermodynamic processes in the ice/atmosphere coupling.

Numerical models offer an alternative approach to air-sea-ice interactions. A major advantage of the modeling approach is the availability of output data for the compilation of mass and energy budgets. However, the behavior of ice as a geophysical fluid is complicated by processes occurring on a wide range of scales. Individual floes, ridges and leads have scales of [10-1000 m], while the large-scale forcing fields are characterized by scales of [100 -1000 km]. Since large-scale associations ultimately represent the integrated effects of small-scale interactions, a sea ice model must be based on an assumed ice rheology through which sub-grid scale processes can be parameterized. The most realistic rheology, used in the modeling work at Illinois (Walsh, Hibler and Ross, 1983), is based on a viscous-plastic constitutive law and an ice strength parameterization. Other essential features of the model are (a) a momentum balance based on geostrophically-derived air and water stresses, Coriolis force, ocean tilt, internal ice stress and inertial terms; (b) an ice thickness, consisting of the a real fraction of open water and one or more thickness categories; and (c) a thermodynamic code in which vertical growth rates are evaluated from heat budget computations at the top and bottom surfaces of the ice and from heat stored in the oceanic boundary layer.

Simulations of ice cover over the Northern Hemisphere oceans have been performed on a 220 km grid (Hibler and Walsh, 1983; Walsh, Hibler and Ross, 1983). The simulations are driven by 20 years of interannually variable forcing fields. However, a 24-hour timestep and daily forcing data must be employed in order to include the short-term fluctuations of the deformation field that determine the areal fractions of open water and thin ice. These areal fractions are the major determinants of the thermal exchanges between the surface and the atmosphere. Considerable mathematical complexity is introduced by the horizontal momentum transfers attributable to the internal ice stress, which requires that a relaxation procedure be used to solve for the ice velocity field at each timestep. Largely because of this relaxation procedure, the model requires approximately 12 minutes of CRAY-1A time per simulated year at the National Center for Atmospheric Research (NCAR).

The present NSF-supported project at Illinois is an effort to determine the physical basis of the multiyear fluctuations which characterize the large-scale Northern Hemisphere sea ice distribution. Preliminary results (Walsh, Hibler and Ross, 1983) show that regional fluctuations of ice *mass* (thickness) have significantly longer time scales than do fluctuations of ice-covered *area.* The conservative nature of the regional mass anomalies have encouraging implications for ice forecasting on the seasonal to annual time scales. When used in conjunction with the model-derived ice velocities, the mass anomalies provide a unique framework for the quantitative description and interpretation of the multiyear fluctuations. Physical explanations of these fluctuations and their evolution are therefore attainable from the model results,

whereas such explanations are beyond the capabilities of observational analyses in the foreseeable future.

Sensitivity tests required for more complete assessments of the model results include the use of temperature/wind forcing data from several sources, experimentation with different numbers of ice thickness categories and with alternative values of the rheology parameters, and an examination of the sensitivities to various elements of the thermodynamic formulation. Since each 20-year simulation consumes 4 CRAY-1A hours, the project will require approximately 100 CRAY-1 or equivalent supercomputer hours for each of the next several years. The saturation of the NCAR CRAY systems has already impeding the progress of the project. When this factor is combined with the expense and delays associated with transfers of large datasets (e.g., 20 years of daily grids) between NCAR and Urbana, the potential advantages of a supercomputing capability at Illinois are considerable.

References

Walsh, J. E., and C. M. Johnson, 1979: An analysis of Arctic sea ice fluctuations, 1953-77. J. Phys. Ocean., *9*, 580-591.

Walsh, J. E., and J. E. Sater, 1981: Monthly and seasonal variability in the ocean-ice-atmosphere system of the North Pacific and North Atlantic. J. Geophys. Res., *86*, 7425-7445.

Hibler, W. D. III, and J. E. Walsh, 1982: On modeling the seasonal and interannual fluctuations of arctic sea ice. J. Phys. Oceanogr., *12*, 1514-1523.

Walsh, J. E., 1983: The role of sea ice in climatic variability: Theories and evidence. Atmosphere-Ocean, *21*, 229-242.

Walsh, J. E, W. D. Hibler III and B. Ross, 1983: A model simulation of twenty years of northern hemisphere sea ice fluctuations. Annals of Glaciology, *5*, in press.

DYNAMICS OF CONVECTION

Robert Wilhelmson - Professor

Department of Atmospheric Sciences

The computer has been an important tool in the Atmospheric Sciences since its development in the early 50's. It continues to be used to help predict tomorrow's weather as well as to study most atmospheric processes. Equations describing fluid flow are integrated in time to study these processes and their relationships with one another. Supercomputers are often used for the integrations because the flow is highly nonlinear and because hours of computer time are often needed just to complete a few simulations. In addition, advice on tomorrow's weather using model predictions is valuable only if it is available before the weather.

The importance of computing power in solving atmospheric problems was recognized at the University of Illinois in the late 60's as plans were laid for enlarging atmospheric research on the University of Illinois campus. As a student in computer science at that time, Wilhelmson worked on software development for ILLIAC IV, a supercomputer which was being designed at the University. Wilhelmson and other atmospheric science faculty made little use of the ILLIAC IV because it was never installed at the University as originally planned. Other computers, however, were used such as the IBM 360/91 at UCLA, the CDC 7600 and more recently the CRAY-1A at the National Center for Atmospheric Research (NCAR).

Wilhelmson has used these computers to simulate convection. The convective studies involve the integration of time dependent sets of equations for fluid flow that yield velocities, temperature, pressure, moisture, and cloud substances (e.g., small drops, raindrops, and hail). The availability of supercomputers during the last 5-10 years has made it possible to carry out many of these simulations in three spatial dimensions. It is important to be able to follow the development of all three components of motion in the simulation of convection such as in storms that produce strong surface winds, hail and tornadoes.

One example of the convective research being pursued by Wilhelmson involves the simulation of severe storms that can produce tornadoes, often known as supercells. These storms possess a distinctive internal circulation that can remain relatively steady for periods of an hour or more once they have formed. A three-dimensional numerical model has been developed in collaboration with Joseph Klemp (NCAR) to not only simulate this quasi-steady structure, but also to simulate in a number of settings the evolution of a small cloud to this state (e.g., Wilhelmson and Klemp, 1978, 1981). In these settings the initial cloud often splits into two storms. One has an updraft that rotates cyclonically (positive vorticity) and moves to the right of the initial storm propagation vector. The other has an updraft that rotates anticyclonically (negative vorticity) and moves to the left. Sometimes, however, only the right or left moving storm forms. It has been possible to use the three-dimensional model to determine how the changes of wind and temperature with height in the storm environment are related to these differences in storm development. This had not been clearly understood before because observed storms often occur in complex environmental settings whereas in the model the setting can be simplified and varied at will.

The model has also been used to augment particular observational case studies of storms. This is an important application since our understanding of storms from observational programs is limited by current observing techniques which do not capture the complete spatial and temporal characteristics of a storm. Modeling, of course, has its own limitations. However, model data sets are more complete. For example, multiple Doppler radar analysis can be used to construct the internal flow field within the precipitation region of a storm, but the temperature and pressure distribution is not directly obtainable as it is in the model.

One recent observational and modeling study was for several tornadic storms that formed in Oklahoma in 1977 (Klemp, Wilhelmson and Ray, 1981). The model storm grew in an environment approximating that observed in vertical structure but was horizontally homogeneous. A number of similarities between the modeled and observed storms were noted, including the rotation of the updraft, the overhang and hook features in the precipitation field and the high surface winds. The observed tornadoes could not be simulated because the model resolution was too course to describe them. However, the dynamics modeled was sufficient for investigating how the rotating updrafts (mesocyclones) in which the tornadoes were

embedded evolved.

It is currently unfeasible to simulate a storm with sufficient resolution to resolve it as well any associated tornadoes, although certain storm characteristics can be simulated using the power of machines such as the CRAY-1A in a reasonable timeframe (up to 2 hours). There are also other storm features such as downbursts associated with some airline crashes and detailed microphysical development that cannot currently be adequately simulated. However, with sufficient computational time available on a supercomputer these phenomena embedded within their parent storms can be studied by increasing the resolution in three-dimensional models. The need for greater computational power is underscored by noting that doubling the number of grid points in a three-dimensional domain implies (using current techniques) a given simulation will take 16 times longer (8 times more grid points and twice as many times steps for numerical stability).

The availability of substantial computer time at the University of Illinois would also allow Wilhelmson together with his students and collaborators to tackle other problems such as how storms interact with other storms and with larger scale systems. This can be accomplished by increasing the integration domain and by other techniques (Wilhelmson and Klemp, 1983; Droegemeier and Wilhelmson, 1983). All these studies will be important for the proposed National Storm Program (A Call to Action, University Corporation for Atmospheric Research, Boulder, Co, 1983) aimed at better observation and prediction of small scale weather phenomena such as thunderstorms, squall lines and flash floods.

A number of atmospheric science faculty and students at the University of Illinois will be participating in this program. Both modeling and observational studies will be continued. In the former, new numerical algorithm development is underway under Wilhelmson's direction to improve resolution of small scale convective features such as tornadoes and downbursts. The interactive graphics and image display system known as VIP (VAX and Image Processing) established in the last few years (primarily by the Departments of Atmospheric Science and Astronomy) will be used for analysis of model and observational data. This system is built around a VAX 11/780 and consists of a number of displays including a COMTAL Vision One/20, Tektronix 4010, 4014 and 4025, an Evans and Sutherland PS 300 realtime vector display and a number of hard copy devices. It's use, plus the availability of a supercomputer, will be important for remaining at the frontier of storm research in terms of both observational analysis and numerical modeling.

Based on current usage of a CRAY-1A at NCAR (about 150 hours/yr), it has been estimated that at least 1000 hours of supercomputer time could easily be used for storm and tornado simulations during the first year the computer becomes available at the University of Illinois. Several convective models currently running on the CRAY-1A at NCAR would be immediately transferred to the supercomputer. Substantial care has already gone into storm model coding so that the full power of a vector machine can be utilized. The main model requires a mass store for saving simulated data for further integration. This is particularly important for long simulations which need to be checked periodically for potential problems. For most simulations, data is swapped between main memory and disk every time step with care to minimize I-O overhead. A solid state disk of at least 32 million words and a large main memory of at least 4 million words would permit higher resolution and large domain simulations to be made efficiently. The code structure is such that it is straight forward to implement changes to utilize both the solid state disk and the other disks as needed.

References

Droegemeier, K. K. and R. B. Wilhelmson, 1983: Three-dimensional numerical simulation of the interaction between a shallow cumulus field and a thunderstorm outflow boundary. *Preprints* , 13th Conference on Severe Local Storms, Amer. Meteor. Soc., Tulsa, OK.

Ericksen, J., and R. Wilhelmson, 1976: Implementation of a convection problems requiring auxiliary storage. ACM Trans. on Math. Software, *2* , 187-195.

Klemp, J. B., and R. Wilhelmson, 1978: Simulations of right and left moving storms through storm splitting. J. Atmos. Sci., *35* , 1097-1100.

Klemp, J. B., R. B. Wilhelmson and P. S. Ray, 1981: Observed and numerically simulated structure of a mature supercell thunderstorm. J. Atmos. Sci., *38*, 1558-1580.

Wilhelmson, R., 1974: The life cycle of a thunderstorm in three dimensions. J. Atmos. Sci., *31*, 1629-1651.

Wilhelmson, R. B., and C. S. Chen, 1982: A simulation of the development of successive cells along a cold outflow boundary. J. Atmos. Sci., *39*, 1466-1483.

Wilhelmson, R., and J. Ericksen, 1977: Direct solutions for Poisson's equation in three dimensions. J. Comput. Phys., 25, 319-331.

Wilhelmson, R., and J. B. Klemp, 1978: A numerical study of storm splitting that leads to long-lived storms. J. Atmos. Sci., 35, 1975-1986.

Wilhelmson, R. B., and J. B. Klemp, 1981: A three-dimensional simulation of splitting severe storms on 3 April 1964. J. Atmos. Sci., *38*, 1581-1600.

Wilhelmson, R. B. and J. B. Klemp, 1983: Numerical simulation of severe storms within lines. *Preprints*, 13th Conference on Severe Local Storms, Amer. Meteor. Soc., Tulsa, OK.

SUPERCOMPUTER ARCHITECTURE, SOFTWARE AND ALGORITHM RESEARCH

David J. Kuck - Professor
Ahmed H. Sameh - Professor
Duncan H. Lawrie - Associate Professor
Daniel D. Gajski - Associate Professor

Department of Computer Science

The Laboratory for Advanced Supercomputers in the Department of Computer Science consists of four regular faculty members (Gajski, Kuck, Lawrie, and Sameh), as well as half a dozen visiting faculty members. Over twenty graduate students are involved. Our activities range from basic studies of parallelism in algorithms to the design of new supercomputer architectures. Our work has had influence (directly or indirectly) on the architecture and software of most of the superspeed systems of the past decade. For example, the CRAY X-MP itself was designed by our former Ph.D. student, Steve Chen, now a CRAY Vice-President. Having a supercomputer on the campus would provide two important kinds of support for us.

First, it would allow us to experiment with various parallel algorithms and compiler strategies for exploiting this system. There are three aspects of the CRAY X-MP or Cyber 2XX that are of interest here.

(1) Vectorization of algorithms and programs to exploit the pipelining of the system [KKLW80], [Kuck81].

(2) Restructuring algorithms and programs for the multiprocessing aspect of the system [KuPa79], [PaKL80].

(3) Memory hierarchy management at three levels: solid state disk, main memory, and vector registers [AbKL81], [ALMY82], [LaRB82].

We have great deal of experience in all three areas and have done some work directly on the CRAY-1S and Cyber 205 concerning points (1) and (3). Having a supercomputer on campus would greatly expedite this work and allow us to continue to study all three points much more effectively than we can at present.

An example of work that is currently under way is the restructuring of a number of standard packages (e.g., EISPACK, LINPACK, FISHPACK, etc.). Our procedure is first to pass a package through our Parafrase system (the most effective automatic restructurer available today). This immediately causes us to add a few assertions about certain programs with poor speedup, rerun them through Parafrase, and than study the results. Those sections of subroutines that will have low degrees of vectorization are rewritten using well-known (or new) parallel algorithms [Gajs81], [GrSa81], [KPSW82], [Same81], and again passed through Parafrase. Our efforts to date have been quite successful in obtaining highly vectorized versions of these standard packages. Parafrase is just beginning to produce good results for multiprocessors as well.

A supercomputer will also encourage interaction between our group and those physicists and engineers on campus who currently consume a large amount of CPU time on the Cyber 175. The fruits of our research will be of great value to them as they modify their numerical algorithms to take advantage of the power of vector and multiprocessor architectures.

The second area in which we need support is in simulating new architectures [WeLa76], [CLYP82], [Gajs81a], [GaSa82], [GaSW82], and in doing numerical error studies [LaSa78], [LaSa80]. This involves large amounts of machine time and is aimed at the study of new system organizations that would be much faster than current supercomputers. For example, we have simulators capable of studying the effects of new memory systems or of new interconnection networks in super-speed multiprocessors. More than half of our

students are involved in such studies. These simulators can be driven directly by the output of Parafrase and hence we would like to carry out massive experiments on all of the 2,500 Fortran benchmarks we currently have.

At this time we are using both the Cyber 175 and IBM 4341, with most of the time on the IBM 4341 (about 1200 hours this past year). And yet, our detailed simulations are made with only several packages (i.e., EISPACK and LINPACK), typically using selected subroutines (perhaps 200 in total) to save time. Thus, to carry out comprehensive experiments for the design of a new computer system and compiler, we would need approximately 10 to 20 times as much machine time as we currently use. This would translate into as much as 200 supercomputer hours per year.

As microelectronic advances allow computer engineers to use more and more components in systems, faster and faster peak performances can be achieved from supercomputers. However, the efficiency of today's supercomputers is often no higher than 10-15%. Our work is aimed at achieving higher efficiencies through powerful restructuring supercompilers and by designing architectures that are well-matched to algorithms. These higher performances would be available to a much wider class of users because our machines are designed to work together with supercompilers.

References

[AbKL81] W. Abu-Sufah, D. J. Kuck, and D. H. Lawrie, "On the Performance Enhancement of Paging Systems Through Program Analysis and Transformations," *IEEE Trans. on Computers,* Vol. C-30, No. 5, pp. 341-356, May 1981.

[ALMY82] W. Abu-Sufah, R. Lee, M. Malkwai, and P. Yew, "Experimental Results on the Paging Behavior of Numerical Programs," Proc. of the 6th Int'l. Conf. on Software Engineering, Tokyo, Japan, pp. 110-117, Sept. 1982.

[CLYP81] P-Y. Chen, D. H. Lawrie, P-C. Yew, and D. A. Padua, "Interconnection Networks Using Shuffles," Special Issue on Interconnection Networks, *IEEE Computer,* Vol. 14, No. 12, pp. 55-64, Dec. 1981.

[Gajs81] D. D. Gajski, "An Algorithm for Solving Linear Recurrence Systems on Parallel and Pipelined Machines," *IEEE Trans. on Computers,* Vol. C-30, No. 3, pp. 209-206, Mar. 1981; also, University of Illinois at Urbana-Champaign, Dept. of Computer Science, Report No. 78-953, Dec. 1978.

[Gajs81a) D. D. Gajski, "Recurrence Semigroups and Their Relation to Data Storage in Fast Recurrence Solvers on Parallel Machines," *Proc. of CONPAR 81, Conf. on Analysing Problem-Classes and Programming for Parallel Computing,* Nurberg, F. R. Germany, pp. 343-357, June 1981.

[GaSa82] D. D. Gajski and A. H. Sameh, "A WSI-Multiprocessor for Iterative Algorithms," *Proc. of the Government Microcircuit Applications GOMAC-82 Conf.,* Orlando, Fl., pp. 166-169, Nov. 1982.

[GaSW82] D. D. Gajski, A. H. Sameh, and J. A. Wisniewski, "Iterative Algorithms for Tridiagonal Matrices on a WSI-Multiprocessor," *Proc. of the 1982 Int'l. Conf. on Parallel Processing,* Bellaire, MI, pp. 82-89, Aug. 1982; Ed. by Batcher, Meilander and Potter.

[GrSa81] J. Grcar and A. Sameh, "On Certain Parallel Toeplitz Linear System Solvers," *SIAM Journ. on Scientific and Statistical Computing,* Vol. 2, No. 2, pp. 238-256, June 1981.

[KKLW80] D. J. Kuck, R. H. Kuhn, B. Leasure, and M. Wolfe, "The Structure of an Advanced Vectorizer for Pipelined Processors," *Proc. of COMPSAC 80, The 4th Int'l. Computer Software and Applications Conf.,* Chicago, IL, pp. 709-715, Oct. 1980.

[KPSW82] D. Kuck, D. Padua, A. Sameh, and M. Wolfe, "Languages and High Performance Computations," Invited paper, *Proc. of the IFIP Working Conf. on The Relationship Between Numerical Computation and*

Programming Languages, Boulder, CO, pp. 205-221, Aug. 1982. (North-Holland); Ed. by J. Reid.

[Kuck81] D. J. Kuck, "Languages and Compilers for Parallel and Pipeline Machines," Invited paper, *Proc. of the CREST Conf. on Design of Numerical Algorithms for Parallel Processing,* Univ. of Bergamo, Bergamo, Italy, June 1981 (Academic Press).

[KuPa79] D. J. Kuck and D. A. Padua, "High-Speed Multiprocessors and Their Compilers," *Proc. of the 1979 Int'l. Conf. on Parallel Processing,* pp. 5-16, Aug. 1979.

[LaRB82] D. H. Lawrie, J. M. Randal, and R. R. Barton, "Simulation of Automatic File Migration Policies," *Proc. of the Fifth IEEE Symp. on Mass Storage Systems,* Boulder, CO, pp. 27-32, Oct. 1982.

[LaSa78] J. Larson and A. Sameh, "Efficient Calculation of the Effects of Roundoff Errors," *ACM Trans. on Mathematical Software,* Vol. 4, No. 3, pp. 228-236, Sept. 1978. [LaSa80] J. L. Larson and A. H. Sameh, "Automatic Error Analysis of Numerical Algorithms--A Relative Error Approach," *Computing,* Vol. 24, pp. 275-297, 1980.

[PaKL80] D. A. Padua, D. J. Kuck, and D. H. Lawrie, "High Speed Multiprocessors and Compilation Techniques," Special Issue on Parallel Processing, *IEEE Trans. on Computers,* Vol. C-29, No. 9, pp. 763-776, Sept. 1980.

[Same81] A. H. Sameh, "Parallel Algorithms in Numerical Linear Algebra," Invited paper, *Proc. of the CREST Conf. on Design of Numerical Algorithms for Parallel Processing,* Univ. of Bergamo, Bergamo Italy, June 1981 (Academic Press).

[WeLa76] K. Y. Wen and D. H. Lawrie, "Effectiveness of Some Processor/Memory Interconnections," *Proc. of the 1976 Int'l. Conf. on Parallel Processing,* pp. 283-292, Aug. 1976.

SEMICONDUCTOR MULTIDIMENSIONAL DEVICE MODELS

Karl Hess - Professor
Nick Holonyak - Professor

Department of Electrical Engineering

Semiconductor device sophistication has reached the point where further advances will require equally sophisticated and complex analytical models. The inclusion of hot electron and small size quantum effects is now mandatory. A current effort in our group is the analytical modeling of the transient operation of Heterojunction Transistors. With the restriction to only a two-dimensional mesh, it will still require 10 hours of CPU time on a Harris 800 computer to determine a pico-second of the device operation, restricting analysis to only short-term effects. A three-dimensional analysis is of course out of the question. The availability of a supercomputer with array-processing power would alleviate these problems. Efficient utilization would lead to a 100 to 1000 speed improvement over the current facilities.

More sophisticated device models which require even longer computation times are currently being developed. In order to accurately predict how a small device will perform it is essential that an ensemble Monte Carlo calculation be made. The ensemble Monte Carlo method determines the behavior of a group or ensemble of electrons as they move through the device. In this way, the current, drift velocity, and carrier energy can all be precisely determined. However, the ensemble Monte Carlo method is extremely complicated for real device simulations. In order to ensure excellent convergence of the statistical estimators of the electron velocity it is necessary to model about 10,000 electrons simultaneously as they move through the device. The behavior of each individual electron must be traced as the ensemble evolves and travels through the device. This requires very high speed performance and extensive memory capacity which is only available on a supercomputer such as the CRAY X-MP. We anticipate using 3-4 hours of supercomputer time per week and that this will greatly enhance the output of our studies. Our usage would start immediately.

References Related to Above Research

(1) T. H. Glisson, J. R. Hauser, M. A. Littlejohn, K. Hess, B. G. Streetman, and H. Shichijo, "Monte Carlo Simulation of Real-Space Electron Transfer in GaAs-AlGaAs Heterostructures," J. Appl. Phys. *51* (10), 5444-5449 (1980).

(2) K. K. Mon and K. Hess, "Electron-Phonon Interaction at Semiconductor Interface," Workshop on Artificial Superlattices, University of Illinois (Oct. 1980).

(3) H. Schichijo, K. Hess, and G. E. Stillman, "Simulation of High Field Transport in GaAs using a Monte Carlo Method and Pseudopotential Band Structures," Applied Physics Letters *38* (2), 89-91 (Jan. 1981).

(4) H. Schichijo and K. Hess, "Band Structure Dependent Transport and Impact Ionization in GaAs," Phys. Rev. B *23*, 4197-4207 (April 1981).

(5) A. Bhattacharyya, B. G. Streetman, and K. Hess, "Theoretical and Experimental Investigation of the Dynamics of Pulsed Laser Annealing," J. of Appl. Phys. *52*, 3611-3617 (May 1981).

(6) H. Kafka and K. Hess, "A Carrier Temperature Model Simulation of a Double-Drift IMPATT Diode," IEEE Trans. on Electron Devices, *ED-28*, 831 (1981).

(7) D. K. Ferry, K. Hess, and P. Vogl, "Physics and Modeling of Submicron Insulated-Gate Field-Effect Transistors. II. Transport in the Quantized Inversion Layer," *Microstructure Science and Technology/VLSI*, pp. 67-104. Norman Einspruch, Editor, (New York: Academic Press, 1981).

(8) K. K. Mon, K. Hess, and John D. Dow, "Deformation Potentials of Superlattices and Interfaces," J.

Vac. Sci. and Technology *19*, 564-566 (1981).

(9) K. Hess and J. D. Dow, "Deformation Potentials of Bulk Semiconductors," Solid State Communications *40*, 371 (1981).

(10) K. Hess, "Lateral Transport in Superlattices, " Proc. 3rd Int. Conf. on Hot Electrons, Montpellier France, 1981.

(11) K. K. Mon and K. Hess, "Resonance Impact Ionization in Superlattices," Solid-State Electronics *25*, 491 (1982).

(12) A. Bhattacharyya, K. Hess, and B. G. Streetman, "Comments on the Plasma Annealing Model to Explain and Dynamics of Pulsed Laser Annealing of Ion-Implanted Silicon," J. Appl. Phys. *53*, 1261 (1982).

(13) K. Hess, J. Y. Tang, K. Brennan, H. Shichijo, and G. E. Stillman, "Reply to Comment on 'Simulation of High-Field Transport in GaAs Using a Monte Carlo Method and Pseudopotential Band Structures' and on 'Band-Structure Dependent Transport and Impact Ionization in GaAs'," J. Appl. Phys. *53*, 3327 (1982).

(14) J. Y. Tang and K. Hess, "Investigation of Near Ballistic Transport Following High Energy Injection," IEEE Trans. on Electron Devices *ED-29*, 1906 (1982).

(15) J. Y. Tang, K. Hess, N. Holonyak, Jr., J. J. Coleman, and P. D. Dapkus, "The Dynamics of Electron-Hole Collection in Quantum Well Heterostructures, J. Appl. Phys. *53*, 6604 (1982).

(16) J. P. Leburton and K. Hess, "Energy Diffusion Equation for an Electron Gas Interacting with Polar Optical Phonons," Phys. Rev. B *26*, 5623 (1982).

(17) K. Hess, "Electron Transport in Heterojunctions and Superlattices," Proc. of the 16th Intl. Conf. on the Physics of Semiconductors, 1982 (invited paper).

(18) J. Dow, S. Y. Ren, and K. Hess, "Random Superstructures," Phys. Rev. B *25*, 6218 (1982).

SIMULATING THE PHYSICS OF TURBULENCE

Tom Hanratty - Shell Distinguished Professor

Chemical Engineering

Present laboratory experimentation on turbulent flows has moved into the direction of multiprobe techniques and conditional sampling. Even with these very complex measurements, not enough information is being obtained to give an understanding of the physics of turbulence. It is becoming quite clear that these laboratory experiments must be coupled with large scale computations which give far more information about the details of a randomly varying field than is attainable in any laboratory experiments. The use of a supercomputer to do experiments with randomly varying velocity and scalar fields is in its infancy. The availability of a supercomputer on the University of Illinois campus would enable us to continue and expand our work in this area.

In recent years, we have been carrying out numerical solutions of the unaveraged Navier Stokes equations and the unaveraged scalar transport equations for randomly varying velocity fields in order to obtain models for wall turbulence consistent with measurements. Solutions of the unaveraged scalar equations have yielded a completely new theoretical approach toward understanding turbulent mass transfer at a solid boundary (1). This was brought about because experiments could be carried out on the computer which were not possible in the laboratory. In particular, by filtering the randomly varying velocity field which was used in the mass balance equation, it was possible to show that only low frequency velocity fluctuations (containing only a small fraction of the energy) control the rate of mass transfer. This work, as well as work on mass transfer at a gas-liquid boundary, is being continued in theses by Eleni Vassiliadou (2) and by Mark McCready (3), as well as in a cooperative research effort with the University of Toulouse.

Our work on numerical solutions of the unaveraged Navier Stokes equations was initially motivated by the discovery of elongated coherent structures in turbulent flows close to a wall. These structures appear to control the transfer of energy from the mean flow to the turbulence and are therefore a key to understanding how turbulence is created. Consequently, our ability to simulate these structures on the computer not only offers the opportunity to solve the problem of wall turbulence, but also offers an experimental system in which one can explore methods for controlling turbulence. In our first work (4) in this area, we solved the unaveraged Navier Stokes equations in the viscous wall region ($40 > y+ > 0$). For simplicity the flow was assumed to be homogeneous in the flow direction. The outer boundary condition was assumed periodic in the direction transverse to the flow (with a wavelength equal to the spanwise scale of the observed wall structures) and periodic in time (with period equal to the lifetime of the wall structures). This simple approach was quite successful in describing many of the main features of the flow close to the wall, and in particular, confirmed that these structures are controlling the transfer of energy from the mean flow to the turbulence.

This success has prompted us to continue this work by considering a more realistic outer boundary condition with velocity components varying randomly in time and in space (5). This work is suggesting important physical processes by which the wall selects certain frequencies and scales. In particular there appears to be a change in the scale of the eddies close to the wall that had not been previously anticipated. We are currently using these models to understand how to affect turbulence by strong pressure gradients (6), by time varying velocity fields (7) and by drag-reducing polymers (2).

This work is focusing our attention on what is probably the key issue in understanding wall turbulence; i.e., the interaction between the viscous wall region and the outer flow. The question as to what governs the physical features of the coherent wall eddies has to be answered. We have been exploring this question by seeing how the wall region responds to different outer boundary conditions. However, this approach is limited because information from laboratory experiments is incomplete.

The correct way to handle this study of the interaction is to do experiments on a computer and not in the laboratory. This would require the modeling of the entire flow field and not just the viscous wall region. Our current work is now reaching the limits of computational facilities on the University of Illinois campus (we use about 35 hrs on the Cyber 175 per year). A large-scale computer of the type outlined in this

proposal would be needed to continue our work in a meaningful way.

Our initial effort would be to extend our present computational domain to cover the whole field and not just the viscous wall region. We would plan to consider fully developed flow in a channel. We could then use just the no-slip condition at the solid boundaries without having to construct complicated outer boundary conditions in order to specify the matching of the wall layer with the outer flow. However, even with a supercomputer it may not be possible to resolve all the important length scales by solving the unaveraged Navier Stokes equations. In our initial efforts, we will use a simplifying assumption which has been quite successful in dealing with the viscous wall region. We will assume the flow to be homogeneous in the flow direction. This would mean the pressure gradient in the flow direction is a constant over the whole flow field and that all derivatives of velocity components in the flow direction (the x-axis) can be related to time variation by using a convection velocity. This greatly simplifies the computations in that they have to be carried out only for a time varying three-dimensional flow field in the y-z plane. Also the x- momentum equation is decoupled from the y- and z-momentum equations. It is realized that the assumption of homogeneity in the flow direction could ignore important physical phenomena. However, our present work indicates that it would retain enough of the general features of a real turbulent flow to define the interaction between the outer flow and the wall layer. After this study is completed, we would then look at how nonhomogeneities in the flow direction influence the turbulence.

Another approach to this problem would be to solve the unaveraged Navier Stokes equations in the viscous wall region, but to use a large eddy simulation model to calculate the outer flow, as was done by a group at the NASA Ames Laboratory. In this case, the computations in the outer flow would be carried out over a three-dimensional rather than a two-dimensional field; however, the grid spacing would be such that all of the small scale turbulence cannot be resolved. Consequently, a closure model is necessary.

During the first year a supercomputer is available we project our use to be about 100 hours as we further develop codes and make initial simulations. This number would then increase substantially, particularly if plans for a larger group of faculty doing turbulent simulations evolves. One such group, formed at the NASA Ames Laboratory, initially used ILLIAC IV for simulating large eddies in turbulent fields (8) (9) (10). We believe that there is a need for several dedicated groups in this country to continue to carry out these types of numerical experiments. The University of Illinois would be an ideal location for such a center for turbulence research, since personnel presently available on campus are sufficient to give the initial impetus that would be needed.

References

(1) J.A. Campbell and T. J. Hanratty, "Mechanism of Turbulent Mass Transfer at a Solid Boundary", AIChE Journal, 221 (1983).

(2) Eleni Vassiliadou, Ph.D. thesis, now in progress, University of Illinois, Urbana.

(3) Mark McCready, Ph.D. thesis, now in progress, University of Illinois, Urbana.

(4) D.T. Hatziavramidis and T. J. Hanratty, "The Representation of the Viscous Wall Region by a Regular Eddy Pattern", J. Fluid Mech., 95, 665 (1979).

(5) Christos Nikolaides, Ph.D. thesis, now in progress, University of Illinois, Urbana.

(6) Douglas Finnicum, Ph.D. thesis, now in progress, University of Illinois, Urbana.

(7) Zhuo-Xiong Mao, Ph.D. thesis, now in progress, University of Illinois, Urbana.

(8) P. Moin, W. C. Reynolds and J. H. Ferziger, "Large Eddy Simulation of Incompressible Turbulent Channel Flow", Report No. TF-12, Thermosciences Division, Department of Mechanical

Engineering, Stanford University, Stanford, California.

(9) J. Kim and P. Moin, "Large Eddy Simulation of Turbulent Channel Flow-Illiac IV Calculation", September, 1979, NASA Tech Memo 78619.

(10) P. Moin and J. Kim, "Numerical Investigation of Turbulent Channel Flow", July, 1981, NASA Tech Memo 81309.

ANALYSIS OF PROBLEMS IN FLOW AND FRACTURE OF STRUCTURAL MATERIALS

Robert M. McMeeking - Associate Professor

Department of Theoretical and Applied Mechanics

Modern structural materials, whether they are metals, ceramics, synthetic composites or polymers, possess complex microstructures which endow the materials with their desirable characteristics. For example, a steel alloy usually has a fine mixture of two or more microconstituents whose complex interactions determine the yield and fracture strength of the material. However, the complexity of the behavior means that the mechanical analysis of processes of failure is relatively difficult and is understood currently only on a qualitative basis or in terms of imprecise quantitative models.

Much progress has been made recently through the use of computers for problems associated with metals, ceramics, composites and polymers but the calculations so far have been only for simple configurations of microconstituents in idealized materials. Access to a supercomputer on reasonable terms would allow us to develop solutions to more realisitc problems and the results will give us more detailed insights into material failure processes. Our ambition is to provide information to material scientists that will allow them to improve the design of the microstructure of materials. Also, the more precise models for failure should give guidance to designers of machines and structures when they set limits to design load or time.

F. A. Leckie (Department of Mechanical and Industrial Engineering and Theoretical and Applied Mechanics) and I have been very interested in problems of ductile and creep rupture. In these problems, the process of failure involves the nucleation, growth and coalescence of holes in metal alloys or ceramics. This process can take place in bulk or can be localized near a stress intensifier such as a crack. The holes are formed around inclusions in the material or at grain boundary imperfections. The inclusions are an inevitable result of the material manufacture. Once formed the holes grow as a result of stress induced plastic deformation due to dislocation motion. At high temperatures (creep) growth can be assisted or dominated by diffusion of material through the grains or along the grain boundaries. Finally, the holes become large enough so that they join together, either by intensification of the deformation between the holes or by rupture of the ligament.

We have achieved some success, as have others (such as A. Needleman at Brown, V. Tvergaard at Odense) in modelling the behavior of individual holes by the finite element method. The finite element method is used to solve by computer the partial differential equations on a grid space and time. Using programs developed by us and by others, we have solved for the behavior of an individual cylindrical hole near a crack tip in tension in an elastic-plastic material and for the behavior of spherical holes in periodic arrays in tension in elastic-plastic materials. The material model is highly idealized, especially as it assumes isotropy and homogeneity. However, these solutions take many hours on the Illinois Cyber 175. It is impossible for us to analyze enough cases to get as much understanding as we would like about the influence of such parameters as inclusion shape, size and spacing. Yet to fully understand the processes, we need to study collections of randomly placed holes of various shapes and sizes as the failure processes gradually develop. These holes should be embedded in more realistic materials than we currently analyze, and the influence of inclusion strength and cohesion should be studied. These compliations mean that we shall need more extensive grids for the solutions which will be based on more complicated non-linear partial differential equations. The increased complexity of the equations will mean that more iterations will be required for convergence. More extensive grids will lead to larger systems of simultaneous equations and large matrices. As a result, the computer calculations will become much more time consuming and expensive on the current generation of machines at Illinois. Going on to study the more realisitc problems will only be feasible for us when we have access to a machine like a CRAY X-MP and I envisage starting at about 100 hours per year and building up from there. Other problems such as ductile crack growth in 3-dimensions on complex paths, the analysis of the development of fatigue and creep damage in materials, strengthening mechanisms in ceramics and failure in metal forming processes are of great interest to us. With a supercomputer we could tackle more useful and realistic problems than we are able to do currently.

Selected References

"On Criteria for J-Dominate of Crack Tip Fields in Large Scale Yielding," with D.M. Parks, ASTM-STP 668, 1979, pp. 175-194.

"Recent Finite Element Studies in Plasticity and Fracture Mechanics," with J. R. Rice, D. M. Parks and E. P. Sorensen, Computer Methods in Applied Mechanics and Engineering, *17/18*, 1979, pp. 411-442.

"Stress and Deformation Analysis of Metal-Forming Processes," with E.H. Lee and R.L. Mallett, Metal Forming Plasticity, Proceedings of IUTAM Symposium (Ed. H. Lippman), Tutzing, W. Germany, 1978, Springer-Verlag, pp. 177-189, 1979.

"Stress and Plane Strain Fields at the Tip of a Stationary Tensile Crack in a Creeping Material," with F. A. Leckie, International Journal of Fracture, *17*, 1981, pp. 467-476.

"Some Effects of Inelastic Constitutive Models on Crack Tip Fields in Steady Quasistatic Growth," with D. M. Parks and P. S. Lam, Advances in Fracture Mechanics, Proceedings of the 5th International Congress on Fracture, Cannes, France, March 1981, Vol. 5, pp. 2607-2614.

"An Incremental Crack Growth Model for High Temperature Rupture in Metals," with F. A. Leckie, Advances in Fracture Mechanics, Proceedings of the 5th International Congress on Fracture, Cannes, France, March, 1981, Vol. 2, pp. 699-704.

"The Generation of Residual Stresses in Metal-Forming Processes," with E. H. Lee, Residual Stress and Stress Relaxation, Proceedings of 28th Sagamore Army Materials Research Conference, Lake Placid, 1981 (ed. E. Kula and V. Weiss) Plenum, New York, pp. 315-330, 1982.

"The Effects of Spherical Voids in an Isotropic Strain Hardening Elastic-Plastic Medium", M. S. Thesis by S. V. Harren, 1983, under R. M. McMeeking.

"Estimates for the Constitutive Moduli of Ductile Materials Containing a Small Volume Fraction of Voids or Inclusions," Mechanics of Materials (D. C. Drucker Anniversary Volume) (eds. G. A. Dvorak and R. T. Shield) Elsevier, Amsterdam, 1983, in press.

FUSION PLASMA ENGINEERING

George Miley - Professor

Department of Nuclear Engineering and Fusion Studies Laboratory

Professor Miley and his colleagues are involved in the development of computational methods for fustion plasma engineering studies [1-2]. This involves the analysis of fusion plasma behavior under realistic conditions expected in future fusion reactors.

In support of this effort, a remote entry job terminal that provides direct access to the CRAY-1, CRAY-1S, and CDC 7600 computers at the National Magnetic Fusion Energy Computer Center (NMFECC) has been located at the University of Illinois. This is on of eleven such units located at universities throughout the country. Professor Miley and his colleagues have been using the NMFECC CRAY extensively through this system since 1978. While this arrangement has been very effective, demands on the LLNL system have gradually increased to the point where time is exceedingly tight. Thus the current allotment of 90 hours CRAY time and 110 hours CDC 7600 time for the Illinois group is only about a third of the time they actually used during the first year of operation of the CRAY. Consequently, the availability of the proposed supercomputer on campus would greatly aid this effort.

A brief review of some of the research recently completed or in progress will illustrate the importance of a supercomputer to this effort.

A variety of new calculational methods are being developed for plasma engineering analysis. These methods typically involve techniques used in basic plasma physics studies, but the application to reactor conditions brings in new demands (e.g. complex geometries and boundary conditions, nonuniform fields, inpurities and neutral gas fluxes) that are frequently omitted in "idealized" plasma physics calculations. These demands in turn force the use of techniques such as multigroup treatments, Monte Carlo, etc.

Multigroup (MG) methods have been developed at Illinois to study fusion product transport and heating [3-4]. The transfer matrix between energy groups is composed of two parts: small energy losses occur via a Coulombic friction term which continuously transfers ions across groups while group skipping occurs through large angle Coulombic scattering (LCS) and nuclear eleastic scattering (NES). The sources term in each group is a sum of ions born via fusion and background "knock-ons" created by LCS and NES events. The solution of the group equation requires an "inner" iteration on the source term each time step.

A variation on the conventional energy-group approach is the dual energy-canonical angular-momentum method employed in the transport code FROST developed at Illinois [5-8]. This code was developed for field-reversed configurations where the complex orbits of high-energy ions (both injected ions and fusion products) affect the net ion current and the internal magnetic field, hence the equilibrium plasma profile.

The calculation of realistic plasma density profiles for magnetically confined plasmas is complicated by the fact that the plasma density profile must be in equilibrium with the magnetic field profile at each time step. This has resulted in the development of the 1 - ½ D plasma-transport method originally proposed by H. Grad at New York University. Basically this involves the solution of the two dimensional Grad-Shafranov equilibrium equation at each time step. Transport coefficients are then averaged over the flux surfaces determined from the equilibrium calculation, permitting a 1-D plasma diffusion calculation.

The Illinois group recently developed an integral transform technique to reduce the computational time required for the 2-D equilibrium calcuation [9-10]. This technique employs a special transform to reduce the partial differential equation which describes the equilibrium with two independent variables to an equation in one independent variable. It is thought that an extension of this technique will make 2 - ½ D calculations practical (i.e. 3-D equilibrium, 2-D transport), and this would be an important step towards more realistic studies of reactor-grade plasmas.

Monte Carlo techniques have been developed at Illinois for several applications such as cyclotron

radiation transport and high-energy ion transport [11-15]. The cyclotron radiation treatment involves a ray-tracing technique with probabilistic decisions applied to scattering-reflection events. Applications to high-energy ion transport are closely related to traditional Monte Carlo studies of charge-particle transport, but, in the fusion plasma case, orbit effects due to the confining magnetic field are included. In order to do this with reasonable computational times, several unique variance reduction techniques are under development [11-14]. Also, a variational technique has been developed that allows plasma stability analysis to be superimposed on the Monte Carlo orbit calculations [17-18].

In summary, the use of a supercomputer for these plasma engineering studies is essential due to the complexity of the problem and the need for realism in modeling reactor conditions. Access to such a computer on campus would greatly accelerate the studies.

References

(1) George H. Miley, "Calculational Methods for Fusion Plasma Engineering," *Topical Meeting on Advances in Reactor Computations*, Salt Lake City, Utah, Vol. II, pp 575-94, 1983.

(2) George H. Miley, "Annual Progress Report, Fusion Plasma Engineerig Studies," Reports C00-2218-216; 238; 295; Fusion Studies Laboratory, U. of Illinois, 1981; 1982; 1983.

(3) J. Galambos, P. Stroud, E. Greenspan, J. Gilligan, and G. H. Miley, "A Multi-Group Method for Ion Slowing-Down with Velocity Diffusion," *Trans. Am. Nucl. Soc., 39,* 490-491, 1981.

(4) J. Galambos, "Ion-Electron Equilibration Power on Advanced-Fuel Burns," *PhD Thesis,* Nuclear Engineering, University of Illinois, 1983.

(5) R. A. Stark and G. H. Miley, "A One-Dimesional Hybrid Code for Field-Reversed Mirror Dynamics," *Bult. APS, 4Z49,* p. 947, New York, 1981.

(6) T. A. Haill, R. A. Stark and G. H. Miley, "A One-Dimensional Kinetic Ion Model for Field Reversed Mirror Dynamics," *Trans. Am. Nucl. Soc., 39,* 491, 1981.

(7) M. Wang and G. H. Miley, "Particle Orbits in Field Reversed Mirrors," *Nuclear Fusion, 19,* pp. 39-50, 1979.

(8) R. Stark and G. H. Miley, "A 1-D Hybrid Code for FRM Start-up," *Trans Am. Nucl. Soc., 43,* 390, 1982.

(9) R. E. Olson and G. H. Miley, "An Integral Transform Technique for Solving the Grad-Shafranov Equilibrium Equation," *Trans. Am. Nucl. Soc., 39,* 489, 1981.

(10) R.E. Olson, "Computational Studies of Ohmic Heating in the Spheromak," *PhD Thesis* , Nuclear Engineering, University of Illinois, 1983.

(11) J. C. DeVeaux and G. H. Miley, "A Variance Reduction Technique for Coulomb-Nuclear Thermalization of Energetic Fusion Products in Hot Plasmas," *Trans. Am. Nucl. Soc., 43,* 393, 1982.

(12) J.C. DeVeaux and G. H. Miley, "Stochastic Transport of High Energy Fusion Products Under Coulomb and Nuclear Scattering in Field Reversed Configurations," *Proceedings of the Sherwood Theory Meeting for Controlled Fusion*, Santa Fe, N.M., Paper #2E39, 1982.

(13) J. C. DeVeaux, E. Greenspan, and G. H. Miley, "Nuclear Elastic Scattering Effects on Fusion Product Transport in the FRM," *Trans. Am. Nucl. Soc., 38,* 215, 1981.

(14) J. C. DeVeaux, "Stochastic Modelling of Fusion Product Transport and Thermalization with Nuclear

Elastic Scattering," *PhD Thesis,* Nuclear Engineering, University of Illinois, 1983.

(15) D. Driemeyer, G. H. Miley, and W. C. Condit, "A Monte Carlo Method for Calculating Fusion Product Behavior in FIeld-Reversed Mirrors," *ANS Topical Meeting Computational Methods in Nuclear Engineering,* Vol. 2, 7-37, 1979.

(16) D.E. Driemeyer, "A Study of Fusion Product Effects in Field-Reversed Mirrors," *PhD Thesis* , Nuclear Engineering Program, University of Illinois, 1980.

(17) E. C. Morse and G. H. Miley, "Stability of the Field-Reversed Mirror," *Nuclear Fusion, 21,* No. 4, pp. 473-479, 1981.

(18) E. C. Morse, "Stability of the Field-Reversed Mirror," *PhD Thesis,* Nuclear Engineering Program, University of Illinois, 1979.

APPENDIX B

GROUP II USERS

RESEARCH PROPOSALS

Brief descriptions of the research interests of the second group of users (see Section IV - Scientific and Engineering Supercomputing) are included in this appendix. Some of these users would use the proposed supercomputer when it becomes available and others would begin to use it over a period of time. A summary of those users currently identified, their department and their research topics can be found in Table 3 in Section IV.

DEPARTMENT OF PHYSICS

Experimental Particle Physics (R. M. Brown)

The Experimental Particle Physics Group currently uses computer time at a rate approximately equivalent to 1000 hours per year on the Cyber 175 for (1) data reduction and analysis, and (2) Monte Carlo and other calculations. Data reduction tends to be I/O intensive, requiring sequential processing of thousands of magnetic tapes while the Monte Carlo calculations are predominantly compute-bound. This computing is being carried out on facilities available through collaborators at national laboratories (Stanford Linear Accelerator Center and Fermi Lab). The Group's dedicated facility on-campus (a VAX 11/780) is principally used for equipment design, small sample data analysis, and program development.

Our data reduction needs require the heavy use of data tapes for which a mass store would be beneficial. Computation-intensive research calculations would be highly valuable and possible on a supercomputer. In particular, design and modeling of new massive experimental detectors requiring extensive CPU time would be possible with faculty and graduate students in residence. This could have significant impact on future experiments open to the Experimental Particle Physics Group. (Members are: G. Ascoli, R.M. Brown, B. Eisenstein, G. Gladding, L. Koester, U. Kruse, T.A. O'Halloran, J. Thaler, A. Wattenberg, J. Wiss).

Light-Energy Transduction in Biomolecules (L. Eisenstein)

The research in my laboratory involves spectroscopic studies of biological chromophores and the proteins to which they are bound. In particular, we are interested in the mechanism of light-energy transduction in biomolecules. Towards this goal we are using Fourier Transform Infrared Difference Spectroscopy to study the rhodopsin (visual pigments) and bacteriorhodopsin systems. We measure changes in the frequencies and intensities of vibrational modes (between 700 and 4900 cm^{-1}) during the process of light-energy transduction. These data have the potential of providing detailed information on the molecular sequence of events and the structural changes in the chromophore, retinal, and protein that follow the absorption of light.

We have already obtained much information from the experimental data using bacteriorhodopsin and rhodopsin reconstituted with retinal analogs with various isotopic substitutions. In order to proceed further in the interpretation of the data, time consuming quantum mechanical calculations on large molecules are required. First, normal mode analysis must be applied in order to correlate the experimentally observed vibrational frequency changes with changes in molecular structure. But in order to be useful, empirically derived force constants must be based on physically meaningful models. We must develop a quantum mechanical theory of force constants. Quantum mechanical calculations of force constants for a large number of different conformations, protein environments, etc., can consume thousands of hours of computer time on a Cyber 175 and only the presence of a supercomputer would make a proper analysis feasible. Second, there is growing availability of structural information about the proteins to which the chromophores are bound and ultimately it would be necessary to use computers to arrive at physically meaningful structures. This can only be accomplished with energy minimizations on systems containing thousands of atoms.

I have begun a collaboration with Barry Honig, Columbia University, on these projects, but we are limited by access to relatively slow computing systems. The availability of a supercomputer at Illinois would not only increase my own commitment to computer based studies, but also it would greatly enhance the collaboration by bringing one of the leading experts in theoretical chemistry to the Urbana campus.

Physics of Biomolecules (H. Frauenfelder)

Biomolecules are complex many-body systems that are specifically designed for certain jobs such as catalysis, storage, or transport of energy, charge, and matter. The exploration of the physics of biomolecules

is in its early stages and we expect that far more experimental data will become available within the next decade and that models and computer simulation will become increasingly sophisticated. While at present the evaluation of our data can be done on smaller computers, we expect computer limitations in a number of areas:

(1) X-ray and EXAFS data evaluation. In collaboration with Petsko at MIT, Parak in Munster (FRG), and Kuntz at UCSF we are expanding the use of X-ray diffraction to study biomolecular dynamics. In our earlier work we have shown that X-ray diffraction can yield information about the mean square deviations of atomic positions (Debye-Waller factor) and hence about motion within proteins. The data evaluation is extremely complex and requires the power of a supercomputer. Work in progress indicates that we can determine the tensor of thermal expansion as a function of position within a protein. Again data evaluation will require extensive computer calculations.

(2) Protein models. In our experimental work we measure simple biological processes, such as the binding of a small molecule to a storage protein, over extended ranges in temperature (2-300 K) and time (ps-ks). The description of such processes requires model calculations that can become very complex since they involve a random walk in a random system. We hope to make our models more realistic and fit our data with these improved models.

(3) Molecular dynamics calculations. Such calculations, based on following the motion of all atoms in a protein starting from the average X-ray structure, have been pioneered by Karplus and collaborators. While we do not perform these computations, we are in close contact with Karplus (Harvard) and McCammon (Houston) to compare their calculations with our data. The work of Karplus and McCammon is severely computer-limited. The presence of a large computer here would move the center of collaboration closer and would attract first-rate theorists.

The availability of significant amounts of supercomputer power at the University of Illinois would have two extremely beneficial effects on our research program. It would allow us to tackle the physics of biomolecules more realistically both through data analysis and theoretical simulations and it would attract additional excellent theorists to our campus who have strong backgrounds in computer methods. The impact of this development on our growing research program should be enormous.

Accretion by Compact Objects and Stellar Dynamics (F. K. Lamb)

Currently one of the frontier areas of astrophysics is the study of time-dependent accretion by strongly magnetic neutron stars and degenerate dwarfs, and by black holes. The study of these flows requires numerical integration of coupled two- or three-dimensional partial differential equations describing temperatures $\sim 10^{12}$ K, magnetic fields $\sim 10^{12}$ G, velocities approaching the speed of light, and very large radiation energy densities. At present, three different types of flows are being modeled, all of which are challenging simulations problem.

First, Keplerian disk flows onto neutron stars (to be extended later to black holes). This is a very wide, two-time-scale problem that involves trans-sonic and trans-Alfvenic flow, modeling of development of the Kelvin-Helmholtz instability, magnetic flux reconnection, and turbulent diffusion. Two- or three-dimensional modeling is essential.

Second, radial flows onto neutron stars. This is also a two-time-scale problem, since the dynamical time and the cooling time typically differ by several orders of magnitude. Simulations must treat the development of Rayleigh-Taylor and Kelvin-Helmholtz instabilities. Two-dimensional modeling is essential.

Third, production of X-rays at the surface of magnetic neutron stars. The complexity of this flow stems from the extreme energy- and angle- dependence of the photon absorption and scattering cross sections, the tight coupling between radiation transport and the hydrodynamics, the two-dimensional geometry, and the necessity of treating particle interactions quantum electrodynamically.

Present efforts on these problems have been limited by the amount of computing time available.

Preliminary exploration of them using one- and two- dimensional codes has required about 40 Cyber 175 hours per year. Efficient progress would probably require at least 100 Cyber 175 hours per problem per year, or a total of 300 Cyber hours, during the first year.

We are also beginning numerical simulations of the dynamical evolution of stellar systems. This is currently another forefront area of astrophysics. The code that will be used interfaces a multi-dimensional Fokker-Planck code, which describes the evolution of the outer regions of the system, with a N-body code that must treat several hundred to a thousand particles in the code of the system. Typical single runs will require 25 Cyber 175 hours. Sample evolutionary calculations would therefore require several hundred hours.

Nuclear Structure and Scattering (D.G. Ravenhall)

Two major areas within nuclear physics are studied by computer here:

(1) Nuclei reactions induced by electrons, and multiphoton corrections to the usual one-exchanged-photon approximations involve the coupling together of several nuclear energy levels. The number of levels which can be included, which determines the degree to which the calculations approach reality, is limited by memory size and time available to some extent.

(2) Calculations of the collective modes of excitation of nuclei using the random-phase approximation become more realistic the more excited the nuclear configurations that can be included. Work with J.P. Blaizot here last semester was very much hindered by the 138K storage limitation of the Cyber. This program is one we hope to continue, along with nuclear experiments.

DEPARTMENT OF ASTRONOMY

Data Processing of VLA Spectral Line Observations (H. R. Dickel)

During the Very Large Array (VLA) Spectral Line Workshop held at the National Radio Astronomy Observatory in 1981, the director presented the "worst case scenario" which dictated the design criteria for VLA processing: 12 hours of 10s integrations using the full VLA (351 individual interferometer pairs), 256 frequency-channels to produce 256 full resolution maps of 2000 by 2000 grid points (4 million per map). In this "worst case," it would take 7.3 hours to read in the visibility data and then computer memory would be completely filled so no further processing would be possible! Therefore current line observations are typically restricted to less than 12 hours of 30s integrations with the possible interferometer pairs, the frequency channels and 1/64 the number of data points per map. Observations of H. Dickel and collaborators have shown that most of the available wealth of detail in the dynamics and clumping of molecular cocoons is missed unless the spatial resolution is 2 arc seconds and the velocity resolution is 0.5 km/s. Except for a few sources, the sensitivity and resolution requirements of such observations necessitate the full VLA and all 256 frequency channels. A supercomputer is needed before the present restrictions can be eased significantly.

Radiation Hydrodynamics of Molecular Cocoons (H.R. Dickel)

After a massive star forms in the dense core of a giant molecular cloud, its ultraviolet radiation ionizes the surrounding medium and an HII region rapidly develops. Eventually, the expanding HII region begins to disperse the inhomogeneous neutral material and clumps may be compressed, resulting in a new generation of stars. Because of the small size of these circumstellar zones, aperture synthesis radio telescope observations are required to map the distribution of various molecules in these sources in order to study the interaction of the ionized flow with the molecular cocoon and to derive the densities, masses and stability of

the clumps. To properly analyze and interpret the data requires theoretical calculations of the dynamical and radiative transfer effects in a clumpy medium. The 2-dimensional, radiation hydrodynamic ("KFIX") code of Sandford and Whitaker at the Los Alamos National Laboratory is the only such one presently available for astrophysical problems. Therefore H. Dickel, in collaboration with Sandford and Whitaker, is applying these calculations to a fragmenting, dense cocoon surrounding a hot, young star and its HII region. One run requires 30 hours using the CDC 7600 computer. In addition, the radiative transfer effects in such a clumpy medium are being explored by means of a slightly modified version of the Kitt Peak National Observatory (KPNO) stellar atmosphere, non-LTE radiative transfer, linear code. One run requires less than an hour on the CDC 7600. Later on, a more powerful (and more computer intensive) Monte Carlo simulation will be performed. A supercomputer at the University of Illinois would not only enable such calculations to be performed here and more quickly, but would also allow development of a more realistic, 3-dimensional treatment.

Chemical Astrophysics (Lewis Snyder)

Observational analysis of data on interstellar molecules is being conducted. The aim of the study is not only to identify these molecules, but also to study their behavior (e.g. shock flows, mass loss). Direct radiative transfer calculations will be undertaken in the study. These calculations are computer intensive and would be carried out on the proposed supercomputer.

Hydrodynamic Studies of Nova Explosions (J. Truran)

It has been demonstrated that common nova eruptions result from thermonuclear explosions occurring in thin accreted hydrogen envelopes on the white dwarf components of binary stellar systems. In particular, hydrodynamic studies have established that, for appropriate choices of initial conditions, the gross characteristics of the early phases of nova outbursts can be reproduced. The restrictive character of some critical assumptions renders it difficult to draw inferences from such studies concerning the long term evolution of nova systems. It is necessary, for example, to include the effects of the very accretion processes which define these systems. The use of very fine zoning is required to provide a realistic measure of the role of radiation pressure in driving wind mass loss. We also note that nova binary systems are characterized by rather short orbital periods (of the order of hours), under which circumstances the two stars are separated by a distance of order a solar radius. During the nova outburst, the companion star can even be engulfed in the extended envelope of the white dwarf. It seems clear that two or three dimensional calculations are appropriate in this case. Here again there is a demand for greater computing power than is currently available at UI.

Explosive Nucleosynthesis (J. Truran)

While the supernova phase constitutes only an extremely small fraction of the lifetimes of a small fraction of all stars, theoretical studies nevertheless suggest that supernova environments provide the setting for the synthesis of most of the heavy elements observed in nature. It is thus of interest to determine the detailed composition of the matter ejected in the explosion of massive stars as supernovae. This necessitates both that the evolution of massive stars be traced through the sequences of nuclear burning phases that occur in their cores and that the nuclear transformations which are a concomitant of the explosive ejection of this core matter be followed. A grand synthesis of stellar evolution, supernova hydrodynamics and nucleosynthesis is thus demanded. Such a study becomes feasible only with more extensive computational facilities than are currently available at Illinois, and thus progress in this area is now being realized only at other research centers.

DEPARTMENT OF CHEMISTRY

Intramolecular Dynamics (J. D. McDonald)

Realistic calculations of intramolecular energy flow in even moderate size molecules (e.g. five to eight atoms) requires large computers. Using small computers (i.e. Cyber 175 class) many groups have done non-quantum mechanical calculations comprising a few trajectories at unrealistically high energies. Some work was done in the mid 1970's on the largest available computer ILLIAC IV by J.D. McDonald. This remains the only work with a statistically significant number of trajectories. What is really needed are calculations on intramolecular energy transfer. These calculations are completely hopeless without the latest generation supercomputers. They would even tax these computers.

Molecular Scattering Theory (D. Secrest)

Most of the interesting results in scattering theory at present are based on approximations of questionable validity. Techniques exist for solving problems exactly; however, they are too computationally expensive or are beyond the power of the computers available at most universities. Theorists working on approximations are working in the dark due to a lack of well understood benchmark calculations which could be used for evaluating the methods. For example, it is known that a number of important phenomena (such as reorientation cross sections resonances and rearrangement reactions) are not treated properly by existing approximations. Extensive accurate calculations must be made before there is any hope of solving these problems since crude model calculations do not work. The availability of massive computing power would make important and basic advances in scattering theory possible. Besides being of great importance to scattering theory, the results of these calculations are of direct interest in astronomy, chemistry and physics.

Collision induced transitions of polyatomic molecules are difficult to study theoretically due to the large number of coupled channels which occur in such collisions. These processes are extremely important in many gas laser systems. The various vibrational states of the polyatomic molecule are coupled through rotation. Each additional vibrational level adds a large number of channels to the scattering equations through its coupling to rotation. Furthermore, it is highly doubtful that the approximations used to treat rotational coupling for diatomics will be useful for polyatomic molecules.

The massive increase in channel coupling will increase the difficulty in solving the close coupling equations by more than an order of magnitude over those for diatomic molecule atom collisions. Many aspects of this calculation may be implemented on a vector machine in a straightforward manner. There are other aspects of the calculation which appear to be amenable to vectorization, though this would require more study.

Along with the close coupling or essentially exact studies on this system we will perform a number of approximate calculations to determine the points of weakness in current approximations. Though large computing facilities will be necessary in carrying out this research, the aim is to develop techniques and approximations which will make it possible to confidently make such calculations using only a modest amount of computing power.

DEPARTMENT OF COMPUTER SCIENCE

Numerical Methods (C. Gear)

Gear has been involved in the development of numerical algorithms and software for the automatic solution of differential equations for many years. In prior years this work has concentrated on ordinary differential equations, particularly in problems with components of many different speeds. When the method of lines is applied to evolutionary partial differential equations, the resulting system of ordinary differential

equations (ODEs) often has components with greatly differing speeds, so some of the methods investigated in prior years have potential for application to partial differential equations (PDEs).

In particular, multirate methods, which can use different steplengths (mesh size) for different components of the system, could permit a more efficient integration of large, time-dependent PDEs in which there is frequent activity in only a few components (corresponding, for example, to the region in which a shock-like transition is occurring). It is also necessary to regrid the space domain (or use something like the moving finite element method) to adapt to regions with rapid transitions. When the method of lines is used, it is necessary to change the number of ODEs dynamically.

Another problem now under investigation for ODEs, that of the efficient use of interative methods to solve the non-linear equations at each step of the integration, is directly applicable to PDEs, because they naturally lead to large, sparse systems of equations that are too large to handle by direct methods.

It is expected that Gear's group will begin to study the application of these ideas to PDEs in the coming three-year period, and could be using about 15 hours on a supercomputer per year by the end of that time.

VLSI Design Automation (W. J. Kubitz and D. D. Gajski)

We are working on the problem of automating the design cycle for digital processors. Our approach allows a high level definition of the processor using a specification language. From this specification, successive hierarchecal decomposition of the data and control paths is performed, using a basic chip floorplan. The decomposition proceeds to a level which allows automatic synthesis of basic cells. The cells are interconnected by abutment to form the chip. There are several computationally intensive tasks which arise in this scheme. These are simulation at the logic and circuit level, some logic and area minimization algorithms, and possibly design rule checking at the mask level.

Iterative Solution of Large Systems of Linear Algebraic Equations (P. Saylor)

My interest is in the iterative solution of $Ax = b$, a universal problem in scientific computation. One hundred thousand equations on one hundred thousand unknowns is roughly the largest set currently feasible to solve. Larger sets will necessarily be solved on a vector or array machine (i.e. on a scientific processor). I advocate a scientific processor for these reasons:

(1) I need to familiarize myself with scientific processors since most of my colleagues outside the university in government or industrial labs use them.

(2) The algorithms I or my students have developed seem to have certain advantages on scientific processors. These machines will therefore become a necessary component of research.

(3) To establish the value of an algorithm it must be tested on matrices provided by industrial or government laboratories. If they are large matrices, a scientific processor may be the only way to solve the equations within a reasonable period of time. Moreover, if comparisons are to mean anything to outside users, the solution should be done on a scientific processor.

Supercomputer Design and Application (D. L. Slotnick)

Research in the design of centrally controlled arrays and other specialized high-performance computing structures makes increasing use of simulation tools. These tools range from gate-level, bit-compatible design simulators to timing simulators useful in estimating algorithm and machine performance. This research also has a growing interface with VLSI design and hence with the CAD/CAM systems that are its

basis. Only the largest scale computers are appropriate to these design and simulation areas.

Simulation of Semiconductor Devices (D. S. Watanabe)

We have developed a package for simulating hot-electron phenomena in short channel MOSFETs. The package is being used to study avalanche breakdown and hot-electron injection into the gate oxide. Both projects should provide important information on the limitations of MOS VLSI scaling. Access to a supercomputer would greatly facilitate this work because our current computing resources are barely adequate for such computationally intensive research. For example, the simulation requires the solution of three coupled nonlinear partial differential equations in two-dimensions and the evaluation of six-fold integrals. A supercomputer would also enable us to extend our research to static three-dimensional and transient two-dimensional problems.

DEPARTMENT OF ATMOSPHERIC SCIENCES

Dynamics of Liquid Drops (K. V. Beard)

The behavior of drops finds numerous applications in the fields of material science, atmospheric science and in technologies associated with sprays and jets (e.g., combustion, painting, printing, inertial fusion). In addition, liquid drop models have been used to simulate such diverse objects as atomic nuclei, biological cells and stars. The mathematical modeling of drop dynamics is complex because of the non-linear nature of fluid inertia and the treatment of a free surface (or its "self-attraction" analog). However spectacular progress has been made using supercomputers to model 3-dimensional nuclear collisions (Los Alamos) and to simulate nuclear dynamics (Livermore). My own research on drop collisions and oscilliation modes could be greatly expanded with ready access to a supercomputer. In particular, the modeling of higher oscillation modes and their affect on average raindrop shape could be extended from 2 to 3-dimensions. This knowledge is essential for interpreting rainfall rates from measurements taken with the most advanced weather radars. Also my work on collision cross sections with rigid-sphere hydrodynamics could be expanded to the more realistic case for deformable drops. The results would fill a large gap in our understanding of how the precipitation spectrum evolves by drop coalescence and breakup. It is clear from the nuclear physics results that 3-dimensional models will provided the "cutting edge" for research in drop dynamics, and that ready access to a supercomputer would allow U of I faculty to participate in such advanced studies.

Climate Modeling (K. Trenberth)

Experiments are planned with a climate model. Such a model incorporates a full three dimensional simulation of the atmosphere and its couplings to the surface of the earth and the oceans. Such couplings go both ways and are very complex in the real world. By controlled experiments with a climate model, certain fields can artificially be held fixed and the effects on the atmosphere and climate system may be isolated. The kinds of experiments planned are as follows: (1) to investigate the role of Antarctica in climate by changing ice sheet parameters; and (2) to investigate the role of regionally concentrated latent heat release in the tropics on setting up wave trains in the atmosphere by artificially constraining the regions where it is released.

DEPARTMENT OF CHEMICAL ENGINEERING

Chemical Process Design (M. A. Stadtherr)

Computer-aided chemical process design (flowsheeting) and optimization may involve the solution of nonlinear equation systems involving thousands, even tens of thousands, of equations and variables. The

traditional approach to solving the problem is to break the very large equation system into many very small systems that are then solved repeatedly until the entire system is converged. For many flowsheeting problems, however, several levels of nested iteration loops arise when this approach is implemented and thus the time required to solve a problem becomes prohibitively large, not to mention expensive. We are pursuing an alternative approach to flowsheeting, iterating on all variables using some sort of simultaneous linearization method. This so-called equation-based approach is much faster than the traditional approach for small to moderate size problems, but for large problems one is often computationally bound by the time and storage required to solve the huge, sparce, linear sub-problems arising during the solution process.

We began about a year ago to consider the use of a supercomputer to break this computational bottleneck. However, flowsheeting matrices do not have the nice structural properties that permit them to be efficiently solved on a supercomputer. Typically, general-purpose sparse matrix routines must be used. Unfortunately general-purpose codes, such as Harwell's MA28, have been shown to be not readily vectorizable and thus there is no great advantage to using them on a supercomputer. If we are to make most effective use of the vector processing power of a supercomputer, we need to rethink the sparse matrix methods currently used for flowsheeting problems. Flowsheeting matrices do have some exploitable structure in this context, namely a bordered block-diagonal or bordered block-triangular structure. We intend to develop and apply the techniques necessary to take advantage of the power of the supercomputer in solving process flowsheeting problems. It is our hope that this will lead to the next generation of techniques for computer-aided chemical process optimization and design.

DEPARTMENT OF ELECTRICAL ENGINEERING

Current Simulation and Design Evaluation (E. Davidson, J. Abraham)

Within our research group, a VAX and HP3000 computer with HP and Tektronix color graphics peripheral stations support LSI circuit design for research with state-of-the-art software. A smaller HP1000 with black and white graphics supports related course work. Computationally intensive tasks such as circuit simulation and design verification and evaluation are extremely limited due to the low speed of these small computers. A supercomputer networked to our system would provide additional capability and would allow designs to be well evaluated prior to fabrication, thereby avoiding costly redesign cycles which can hurt our research effort.

Inverse Problems in High Resolution Image Reconstruction (W.K. Jenkins)

We are involved in the study of high resolution image reconstruction from various types of remotely sensed data. Three particular problems of interest, which fall within the general class of inverse problems, are computer-aided tomography, synthetic aperture radar, and sonar beam forming. These are three rather different problem areas that are related by means of a common theory of signal processing for synthetic resolution. These problems typically involve huge quantities of multidimensional data, require large amounts of computing resources, and have as an ultimate goal real time processing speeds. Up to now, our ability to do extensive experimental research on these problems has been limited by computer costs, computer speed, or memory limits. The addition of a very high speed computer on campus would enhance our ability to carry on and expand our research in the area of inverse problems.

Evaluation and Design of Communication Systems (M. B. Pursley)

A typical example of a situation where the cost or availability of existing facilities is the limiting factor in our research activities is the design and performance evaluation of digital communications systems. For even moderately complex system models it may be possible to obtain only suboptimal design criteria and unacceptably loose bounds on system performance using analytical techniques. In such situations it may, for example, be desirable to perform an exhaustive search for an optimal set of transmitted signals and/or evaluate the probability of incorrect reception by means of a many-fold numerical integration. However, in

many cases of practical interest neither an optimization of signal sets nor an exact evaluation of the key system performance parameters is feasible due to limits on the expense and/or availability of processor time. The ability to optimize and accurately evaluate more complex digital communications systems would be very useful and the subsequent results would almost certainly provide insight for the development of new analytical techniques applicable to the design and analysis of more complex systems.

DEPARTMENT OF MECHANICAL AND INDUSTRIAL ENGINEERING

General Radiation Transport Computations (R. O. Buckius)

General infrared radiation calculations play an important role in energy transport analysis. Many of the gaseous species present in a medium contribute to the emission and absorption of infrared radiation. When the medium contains local inhomogeneities, such as particles or voids, consideration must be given to scattering. The relative contributions of absorption, emission and scattering depend upon the specific application. The computational difficulties that arise in scattering problems are due to the two domains on which radiation calculations depend -- wavenumber and space. Infrared radiation through gases and/or particulates is wavenumber dependent by the nature of their absorption and emission processes. The absorption and emission of infrared radiation by gases is associated with the energy level transitions of the molecules of the gas and, therefore is, very wavenumber dependent. The absorption and scattering processes for particulates are much different from those of a gas. The absorption and scattering varies continuously with respect to wavenumber. The dependence of the radiation properties on a single space dimensional introduces a significant complication and inclusion of higher space dimensions has not even been attempted.

The "standard" method in solving radiative transfer problems, where there are rapid changes in the absorption spectrum and significant scattering contributions, is to solve the equation of transfer for each wavenumber and integrate over all wavenumbers. An alternative approach has been developed to determine all the possible path lengths of all the photons in a conservative scattering medium and then with the path lengths, determine the transfer with absorption. The scattering characteristics for a conservative scattering medium are specified and the distribution of path lengths is determined for a specified source and observer. Once the unique path length distribution has been determined for the specified conditions, absorption effects are included since the absorption depends only upon the length of photon travel. The path length approach enables the absorption and scattering effects to be completely separated. This approach coupled with efficient numerical techniques has been applied to one-dimensional radiation transfer problems. The computational advantages over the "standard" method are significant.

The one-dimensional results that have been obtained to date are computer limited on our present machine. The results do not include the wavenumber dependence of the scattering properties, the spacial dependence of all properties, the multi-dimensional transport dependence or coupling with other modes of energy transport. Multidimensional extensions of the above analysis impose very severe size problems when only the radiation transport is included. If computations of multidimensional radiation transport coupled with large scale convective transport models are to be possible, a supercomputer is required.

Modeling of Gas Dynamics (W. L. Chow)

The problems encountered in our gas dynamic research vary from transonic inviscid-viscid interaction flows to the Navier-Stokes turbulence flows. Under many occasions, due to the insufficient memory on the Cyber 175, we must carry out computations in segments and completion of one case usually requires a few days for handling input and output of intermediate calculations. When solving for flow past an airfoil with a large angle of attack, the modeled suction peak pressure at the leading edge does not compare well with the experimental data and this appears to be related to insufficient memory in the calculation. We have never attempted any three-dimensional flow problems nor have we attempted to solve steady flow problems on the basis of initially unsteady flow due to limitations of our computing facilities. Improvement of our computing facility would definitely improve our position of research in these areas.

Hydrodynamic Shock Physics (H. Krier)

Our work involves modeling stress wave propagation through homogeneous and heterogeneous reactive materials. In particular, we are interested in the hazard of Deflagration to Detonation Transition (DDT), a possibility when solid rocket propellant is ignited in a confined region. In brief, the DDT process is a coalescence of propagating stress waves into a shock front which then shock initiates the remaining material. Since the time scale of DDT is of the order of microseconds and the detonation pressures obtained in the hundreds of kbar (100,000 atms), accurate numerical models of the process are a necessity in trying to understand the physics involved. At the present time, local computing capabilities limit our numerical models to course one-dimensional wave codes. Solving the more realistic two and three dimensional wave propagation problems requires a computer with both increased core memory as well as computing speed.

3-D Flow Fields in Combustion Chambers (H. Krier, J. E. Peters)

The flow fields resulting in high throughput combustor chambers are complex and three-dimensional. The injection of a liquid fuel sets up vortices which alter the turbulent nature of the reacting flow into discrete recirculating zones. Only with the power of a supercomputer would it be possible to model the processes involved in such combustors. The prediction of turbulent mixing and energy-release rates with actual (not ideal) flow conditions will contribute significantly to the efficient use of fuels and to the minimization of pollutant formation. To date no such calculations (solving two-phase, reacting, turbulent flows, in 3 dimensions) are available due to the insufficient speed and storage space of existing computers.

DEPARTMENT OF THEOREICAL AND APPLIED MECHANICS

Comparison of Simulated Turbulence with Experiment (R. Adrian)

A supercomputer center would constitute a quantum jump in our research capability that would have significant scientific benefits on a national scale. In the area of turbulence research, large numerical solutions of the unaveraged turbulent Navier-Stokes equation provide huge data bases that contain far more information on the physics of turbulent flow than any experiment we can conceive of today. Thus, numerical experiments in turbulence have become one of the foremost tools for turbulence research, and they are supplanting physical experiments in many areas. Large numerical turbulence studies are limited to a handful of research groups presently, i.e., NASA Ames--Stanford, Cornell, MIT and NCAR, and there is a clear need for more research groups in this area. I believe that Professor Hanratty's suggestion for a Center for Turbulent Flow Calculations based on the availability of a supercomputer is an excellent idea in this regard (see Appendix A). I would be interested in participating in the formation and operation of such a center.

My personal research interests lie in the experimental study of the physics of turbulent flow, but I have followed the progress of numerical experiments as a means of pursuing these studies for a number of years. During the spring of 1982 I spent a sabbatical period at Stanford where I studied the work that had been done by Professors Reynolds, Kim and Ferziger on the Illiac IV at NASA Ames. I also visited with Dr. Leonard and Dr. Moin at Ames and acquainted myself with their work. Presently, I am negotiating a two year grant with NASA Ames in which we would use one-dimensional solutions of Burgers' equation as data bases for the study of proper orthogonal decomposition and characteristic eddy techniques used in the statistical description of turbulence. This grant will provide an entry into numerical turbulence work which could be upgraded sensibly to three-dimensional studies if a supercomputer were available.

The groups at Stanford and NASA Ames have been working with a Cray computer for almost two years and have developed a considerable body of software for Cray applications. The availability of this software, including I believe some special vector oriented compilers, would argue in favor of a Cray computer for our campus.

System Identification and Reliability (L. A. Bergman)

Basically, I am involved in identification of fundamental system parameters given response data. Computationally, it is a filtering problem that requires solution of large systems of non-linear evolutionary equations. For large, complex structures such as offshore towers, systems of 100,000 equations are likely. The payoff is early detection of system failure. We've had some success computing conditional probabilities of failure of large complex structures through numerical solution over a safe domain of a class of initial-boundary value problems, one equation for each mode of the structure. This in itself would be greatly enhanced by better facilities. However, the final answer requires an additional integration over all possible safe domains sampled from a given distribution. Such calculations on a supercomputer would truly be breakthrough results.

DEPARTMENT OF CIVIL ENGINEERING

Structural Optimization (R. Haber)

Computer-aided design of structural systems for both mechanical and civil engineering applications is already becoming commonplace in industry. At present, the computer is used mainly to evaluate design solutions proposed by a human designer and to help manage the volumninous data associated with these designs. It is clear that in the future the computer will play a more active role in the synthesis of structural forms and in the refinement and optimization of their properties. Although computer methods already exist to address these issues, their use has been limited due to the very large computations required. For this reason, it has only been possible to investigate the influence of a limited number of design parameters on relatively simple structures. A machine with very large memory capacity and very high speed would permit these methods to be applied to practical design problems.

Structural Mechanics (L. A. Lopez)

Current research in civil engineering structures is focused on large scale simulation of real systems. The detail needed to model complex components for both linear and nonlinear material behaviors subjected to a variety of environments such as earthquakes, tornadoes, high winds, etc. has led to heavy dependence on the finite element method of analysis. Today, the method's applicability is limited only by the availability of computing power. In the next generation of research we will not only be developing the method, but also applying it to new and different engineering problems. These problems will be one to two orders of magnitude larger than the ones currently being examined. Artificial limits peculiar to one current generation of computers such as memory size limitations, low data rates, and lack of adequate graphical devices prevent us from even considering some aspects of research in this area.

Computer Aided Design/Computer Aided Manufacturing (L. A. Lopez)

Analysis is only a small part of design, our final product in engineering. The effective use of the finite element method as part of the computer aided design (CAD) process requires the integration of graphics, expert systems, database management, and many phases of engineering technology. In order to carry out integrated approaches to the designs of the future, it is necessary to begin to use a distributed processing approach to computing. Powerful engineering work stations which will have the power of what many people consider today to be mainframe computers will be needed as the man-machine interface. These local work stations must be backed by a large supercomputer to perform the analyses described earlier. In order for this approach to be effective, data transfers between the two types of equipment must be extremely fast and transparent to the user; they must be such that entire databases can be transmitted in a very short period of time. Breakthroughs in this new level of integrated design technology are not possible until the proper kind of equipment is available at the University.

Groundwater Contamination (A. J. Valocchi)

In recent years, finite difference and finite element techniques have been widely used to study the transport of pollutants through groundwater aquifers. However, due to computational limitations, these analyses have been restricted to relatively simple one- or two-dimensional computations. Naturally occurring soils are both heterogeneous and three-dimensional; moreover, many important contaminants undergo complex, nonlinear chemical and biological transformations. Also, the governing equations for pollutant transport through unsaturated soils are highly nonlinear and their solution is extremely difficult and time consuming. A high speed supercomputer with large central memory would enable us to study these more realistic problems.

DEPARTMENT OF AERONAUTICAL AND ASTRONAUTICAL ENGINEERING

Computational Gas and Fluid Dynamics (S. M. Yen)

The objectives of the research programs in computational gas and fluid dynamics under Yen are to develop numerical methods to solve nonlinear gas and fluid dynamic problems characterized by complexities in flow conditions, boundary conditions and flow geometry and to study the flow characteristics of these problems. Further advances in the research efforts depend critically on the availability of a supercomputer.

Specifically, there are three research programs in computational gas and fluid dynamics. All three programs are distinguished by the use of unique and accurate numerical methods developed at Illinois.

(1) In the Boltzmann research, a Monte Carlo method is used to simulate accurately the inter-molecular collision phenomenon. It is basic in determining the gas behavior in a system far from thermal equilibrium. The direct solution of the nonlinear Boltzman equation for multi-dimensional problems, which was considered for many years as impossible, has received increasing attention in recent years. There are two requirements for implementing this method in a large flow field: an accurate Monte Carlo method (which we have) and a supercomputer (which we do not).

(2) Nonlinear free surface wave problems are considered to be one of the important areas in fluid dynamics in which the understanding of the complex wave interactions depends on the study and analysis of detailed numerical solutions. Yen has recently been engaged in developing numerical methods to deal with computational difficulties characteristic of these problems. The implementation of these methods in three-dimensional problems requires the use of a supercomputer with a core memory of at least 2 million words.

(3) The aerospace industry has a keen interest in the use of computers to design aerospace vehicles. Such a task is possible only after accurate computational methods are developed for three dimensional flow. Yen has worked closely with people in NASA/Ames Research Laboratory in the development of these methods. At present, the study is limited to consideration of an ideal (inviscid) gas on the NASA Ames CRAY 1 (with 1 million words of core memory and 8 million of extended memory which allows a computational mesh sixe of 130x30x20). Increased resolution is needed to handle the large change in properties encountered in non-ideal (inviscid) flows. Thus, it would be advantageous to use a supercomputer with larger main and extended memories.

DEPARTMENT OF BIOLOGICAL SCIENCES

Biomechanics of Cell Sheets (J. Mittenthal)

In the development of animal embryos one of the most important processes is the shaping of sheets of cells. Cell sheets, or epithelia, thicken and fold in early stages of development of the central nervous system, of the special sensory organs (eye, ear, nose), and of many internal organs (lungs, liver, pancreas, kidney). We do not understand how forces are generated, and how they act to make epithelia thicken and fold. I am developing a theory for this process, in collaboration with Dr. Robert McMeeking of the Department of Theoretical and Applied Mechanics. The theory allows analysis of the ways in which differential adhesion among cells, and regional differences in the mechanical stiffness of the epithelium, can determine its shape -- the global distribution of its curvatures, thickness, and cell shapes. Our analysis proceeds from the theory of elastic shells in continuum mechanics. However, to accomodate the behavior of cell sheets we have modified this theory to treat the epithelium as a sheet which bends elastically but can undergo fluid-like in-plane rearrangement of cells. For non-axisymmetric cases, finite element methods require that very large arrays of data be processed iteratively, with many repetitions, until convergence to a stable solution is attained. Calculation of transients in this system will require even more extensive computation. Therefore, I can foresee making good use of a new supercomputer on the UI campus.

Simulation of Living Cells (R. P. Futrelle)

The research in my laboratory centers on the behavior of living cells during embryonic development. Over the past few years, I have been developing a mathematical model of signal processing and locomotion of cells which we have simulated on a computer. The model is a great step forward in cell biology, but as currently implemented it is quite schematic, approximate and incomplete. Even with the VAX computer we are acquiring for our laboratory, I estimate that it will not be practical to run a properly fleshed-out version of the model because we will need to solve multicomponent nonlinear parabolic equations on a 3-D grid of $>$ 100,000 points over many, many iterations. Our VAX would give turn-around times of 100's of hours for each example studied, limiting the insight we could gain and keeping a damper on our productivity. The results are also best viewed on a rather sophisticated high-performance color display (which we don't have) in order to understand them properly. The only answer to these challenges is a supercomputer facility.

Emergent Oscillatory Properties of Neural Networks (E. Jakobsson)

From computations with a small number of simulated neurons (using a modified Hodgkin-Huxley membrane model), we have found that neural networks may have a sustained oscillatory output even though none of the cells individually do, provided the cells form a cyclic network connected by unidirectional synapses. This raises the question as to whether circadian rhythms and other important biological oscillations may arise automatically in large interconnected networks of excitable cells functionally connected by chemical transmission. Because of the nonlinear character of these systems, direct simulation is indicated. Access to a supercomputer is needed to do realistic simulations on a large enough network of excitable cells to test this point. A second issue to be explored by such computation (at the other end of the systems dynamic timescale) is the basis for the apparently holographic characteristics of memory storage in the visual cortex. The question is whether synapse modification in a large network associated with experience might give rise to some periodic properties analogous to the wave interference patterns embedded in a holograph. Large network simulations would be necessary to see such patterns in the simulated neural behavior, for the same reasons that large holographs give clearer pictures than smaller ones.

DEPARTMENT OF ACCOUNTANCY

Multiple Time Series Analysis (J. McKeown)

Multiple time series analysis is a means of simultaneously considering a set of interdependent variables. There are many examples of this sort of situation in economic (and other) processes. One of the primary difficulties with the application of multiple time series is that it is a vector process whose dimensions grow rapidly as the number of variables and number of observations increase. The latter is a particular problem in that the researcher is always striving to include as long a time series as possible to facilitate identification and estimation. A further computational drain is that many of the variables require simultaneous estimation of transformation parameters. Within the foreseeable future I expect to see development of the methodology of cross-sectional simultaneous estimation of multiple time series processes.

APPENDIX C

HISTORICAL SKETCH OF SUPERCOMPUTING AT ILLINOIS AND CURRENT CAMPUS COMPUTING

The University of Illinois has a long history in computer development and operation. Supercomputers, defined as the largest and fastest computers available, have been part of this history extending back some 35 years. The first machine and supercomputer in its time was designed and built for the Army in the Digital Computer Laboratory (DCL) in the late 1940's and early 1950's. ORDVAC, as it was called, was generally similar in design to the vonNeumann machine at Princeton and it acutally became operational before the Princeton machine.

The ORDVAC was followed closely by a second system called ILLIAC I (Illinois Integrator And Computer). This machine was one of the first electronic computers both built and owned by an educational institution. It was in operation for ten years and from among many projects was used to design research instruments such as high-energy particle accelerators and the University's radio telescope.

In the late 1950's ILLIAC II was designed and built in DCL. This system paved the way for many innovations in parallel processing in the IBM STRETCH Project (e.g. interleaved memory, pipelined instruction processing, etc.). It performed an addition in two microseconds and a multiplication in six microseconds. In the completion of its first major test, an hour long problem in gas dynamics, half a billion arithmetic operations were performed.

The ILLIAC III project was initiated in the mid-60's. Sophisticated input and output devices were developed to digitize images and display then in various ways. Although commonplace today, these devices were among the first ones of their kind developed.

The ILLIAC IV was also designed during the mid 1960's in the new Computer Science Department at the University of Illinois. Initial plans indicated that it would by far be the largest and fastest computer in the world. A joint effort between the University and the computer industry eventually let to the construction of ILLIAC IV by Burroughs in Paoli, Pennsylvania. It was installed at NASA Ames Research Laboratory in California. This supercomputer, with 64 individual processing units linked together, was used by some faculty at the University of Illinois and its development and use led to increased interest in parallel processing.

Since the time of ILLIAC I scientists and engineers at the University of Illinois have been extensive users of supercomputers at Illinois and elsewhere. Some faculty have also been involved in the development of numerical algorithms and software systems for these machines, some of which have been widely used. Through the 1970's most of the supercomputing by Illinois faculty has been done at national laboratories since a supercomputer was not available on campus.

A strong group of supercomputer designers has been active for some years in the Laboratory for Advanced Supercomputers of the Department of Computer Science. They are currently designing the Cedar multiprocessor system. A prototype of this system should be operational in about three years. This system is based on some new principles in high-speed computing, and will be used experimentally by University of Illinois scientists and engineers.

The present computing environment at Illinois can be broken down into four major parts. Administrative computing is a University-wide service operated under the Vice President for Business. Computer assisted instruction programs are operated by the PLATO group. Most of the student computing, and about half of the research computing, is provided by the Computing Services Office (CSO). The remaining computational resources for research are provided by a large collection of departmental or project oriented systems.

CSO was created in the early 1970's, after about 20 years of computing supervision by the Digital

Computer Laboratory and subsequently the Department of Computer Science. CSO now operates two large CDC Cyber 170's, two IBM 4341's and a DEC VAX 11/780. A network of about 300 public terminals and 125 dialup lines provides user access, along with 12 printer stations located around the campus. Recent activities at CSO have centered around incorporation of a CDC Mass Storage System and development of a campus wide coaxial cable system for data. This year CSO will be installing the first phase of a Hyperchannel for interconnecting its multiple systems as well as beginning to open up high speed interconnection with other campus systems. CSO supports approximately 20,000 users and is 70% funded by direct campus support.

The campus policy on computing reflects a desire to provide an effective environment for computing and does not encourage either centralization or decentralization of resources. It has long been recognized that the diverse needs can best be met by both types of facilities depending on the special needs of individual projects and the special funding opportunities available. Many departments or projects have their own computational resources, as mentioned earlier. Some of these have evolved over the last 10-15 years. Incorporating recent developments in networking in order to connect the various facilities makes the campus policy even more effective.

Major examples of dedicated facilities include:

Biology	VAX
Chemistry	2 VAX's
Civil Engineering	Burroughs B6700 and 4 Apollo's
Computer Science	Prime, 9 VAX's plus many specialized graphics devices and workstations
Electrical Engineering	Harris
Materials Research Lab	4 VAX's plus FPS-164
Astronomy, Atmospheric Sciences, CSO	VAX and Image Processing System
Physics - Betatron	Perkins Elmer
Physics - High Energy	PDP-1060, VAX
Psychology	Harris
Survey Research Lab	PDP-11/70

In addition, there are over 100 LSI-11 systems, 400 personal computers,and a range of older PDP-11 based systems.

There has been substantial interaction between dedicated computer facilities and CSO including maintenance, configuration assistance, software acquisition and distribution, and communications planning. Increasing emphasis is going into networking and network services, equipment evaluation, and facilities management. In addition there have been several joint research efforts, particularly in the area of managing massive file systems.

Planning is underway for major growth in computing activity on the Illinois campus. Access to a limited amount of campus supported computing is currently available to all students and faculty. Plans call for raising these limits dramatically in the future as well as for making more services available. Given the high degree of local familiarity with computing, this growth will only be limited by the ability to finance services.

One unusual feature of computing at Illinois has been the focus on large problems. Since 1975 there has been a policy of taking the time that would otherwise go unused due to daily, weekly and seasonal variation in demand, and making it available to a few large projects. Each CSO machine has about 1200-1500 hours per year that is made available in this way, and there are usually about 10 active projects. This has allowed a few projects to be undertaken that otherwise might not have been attempted. The most widely recognized effort to date has been the successful proof of the Four Color Theorem (Appel and Haken). Some other efforts have been in the areas of computer architecture (Kuck), stellar evolution (Iben), chemical chromodynamics (Dykstra), gauge theory (Kogut), fracture of structural materials (McMeeking) and analysis of the brownian motion of ions in membrane channels (Jakobsson).

APPENDIX D

VITA'S OF THE PRINCIPALS INVESTIGATORS

VITA AND BIBLIOGRAPHY

LARRY L. SMARR

PRESENT POSITION: Associate Professor, Astronomy and Physics Departments, August 1981-present

PREVIOUS POSITIONS: Assistant Professor, Astronomy Department, August 1979-August 1981, and Physics Department, August 1980-August 1981, University of Illinois at Urbana

Junior Fellow, Harvard Society of Fellows; in Departments of Physics and Astronomy, Harvard University, August 1976-July 1979

and Research Affiliate, Department of Physics, Yale University, September 1978-July 1979

Research Associate, Princeton University Observatory, July 1975-July 1976

Lecturer, Department of Astrophysical Sciences, Princeton University, September 1974-June 1975

Research Assistant, University of Texas at Austin, Physics Department (1972-1974); Stanford University, Physics Department (1970-1971)

NSF Predoctoral Fellow - University of Texas at Austin (1972-1973), Stanford University (1970-1971)

OTHER PROFESSIONAL EXPERIENCE:

Consultant to Lawrence Livermore Laboratories (December 1976-present)

Physicist, "B" Division, Lawrence Livermore Laboratories (summer 1976, 1977, 1978, 1979)

Consultant to Smithsonian Astrophysical Observatory (July 1979-1981)

Associate Editor: J. Computational Physics (1977-1980)

Participant in NSF Retreat on Computers for Research (May 23, 1983)

Member, NSF Subcommittee on Computational Facitilies for Theoretical Research (March 1981). Published Report to Advisory Committee for Physics.

Executive Committee, World Space Center (1977-1980)

Co-Founder (Nov. 1981) and Co-Director, Illinois Alliance to Prevent Nucear War

EDUCATION:

University of Texas at Austin	Ph.D.	January 1975
Stanford University	M.S.	January 1972
University of Missouri	M.S.	August 1970
University of Missouri	B.A.	June 1970

Ph.D. Advisor: Bryce S. DeWitt
Ph.D. Title: The Structure of General Relativity with A Numerical Illustration: The Collision of Two Black Holes (copies available on request)

STATISTICS: Born October 16, 1948; married; two children.

AWARDS AND HONORS:

Max-Planck Institute for Physics and Astrophysics Fellowship (summers 1982, 1983)

Alfred P. Sloan Research Fellow (1980-present)

Listed in American Men and Women of Science

NSF International Travel Grant (1974) to Israel

Lane Scholar (1973-1974) - outstanding work in classical physics at University of Texas

National Science Foundation Fellow (1970-1973)

Woodrow Wilson Independent Study Award (1971) - top 10% of Woodrow Wilson Fellows

Woodrow Wilson Fellow (1970)

Honorary Societies:
- Phi Beta Kappa (Scholastic)
- Sigma Xi (Science)
- Sigma Pi Sigma (Physics)
- Pi Mu Epsilon (Mathematics)
- Omicron Delta Kappa (Leadership)
- Phi Kappa Phi (Scholastic)

PROFESSIONAL SOCIETIES & COMMITTEES:

Member, American Association for the Advancement of Science
Member, American Physical Society
Member, American Astronomical Society
Member, International Society on General Relativity and Gravitation

EXTENDED VISITS AS GUEST SCIENTIST:

Max-Planck Institut for Astrophysics, Munich - June 1981, July 1982, July-Aug. 1983

Nordita, Copenhagen - May 1981

Institute of Astrophysics, Cambridge, England - May 1980 & Easter Term 1978

Lawrence Livermore National Lab., Livermore - summers 1976-1981

Princeton University Physics Dept., Princeton - May 1971 & 1972

UN Institute for Theoretical Physics, Trieste - July 1971

OBSERVATIONAL FACILITIES USED AS GUEST SCIENTIST:

Einstein x-ray telescope (with van Speybroeck, et al.)

KPNO 2.1-m optical telescope with video camera
- Oct. 1980 with A. Wirth and J. Gallagher

VLA radio interferometer - August 1981 with R. Ekers
- September 1981 with R. Hjellming & L. van Speybroeck
- Fall 1982 with R. Ekers, D. Sumi, & T. Cornwell

Multiple Mirror Telescope
- Fall 1982 with A. Wirth & L. van Speybroeck

COMPUTATIONAL FACILITIES USED AS GUEST SCIENTIST:

Lawrence Livermore National Laboratory: CDC7600, 1976-1981
CRAY 1, 1981, 1982, 1983

Max Planck Institut fur Astrophysik: CRAY 1, 1981, 1982

CURRENT GRANTS:

NSF Research Grant $547,389 over 4 years

NSF Equipment Grant $151,000 over 2 years

A.P. Sloan Fellowship $20,000

PUBLICATIONS

Professional Articles

(published or submitted for publication)

1. "Surface Geometry of Charged Rotating Black Holes," Phys. Rev., D7, 289, 1973.

2. "Mass Formula for Kerr Black Holes," Phys. Rev. Lett., 30, 71, 1973.

3. "Maximally Slicing a Black Hole," Phys. Rev., D7, 2814, 1973, with S. Christensen, B. DeWitt, F. Estabrook, E. Tsiang, H. Wahlquist.

4. "Mechanism for Inducing Synchronous Rotation and Small Eccentricity in Close Binary Systems," Ap.J.(Lett.), 202, L135, 1975, with W.H. Press and P. Wiita.

5. "The Binary Pulsar -- Physical Processes, Possible Companions, and Evolutionary Histories," Ap.J., 207, 574, 1976, with R. Blandford.

6. "Collision of Two Black Holes: Theoretical Framework," Phys. Rev., D14, 2443 (1976), with A. Cadez, B. DeWitt, K. Eppley.

7. "Gravitational Radiation from Distant Encounters and Head-On Collisions of Black Holes: The Zero Frequency Limit," Phys. Rev., D15, 2069, 1977.

8. "Spacetimes Generated by Computers: Black Holes with Gravitational Radiation," Ann. N.Y. Acad. of Sciences, 302, 569, 1977.

9. "Are There Geon Analogues in Sourceless Gauge-Field Theories?," Comm. Math. Phys., 56, 1, 1977, with S. Coleman.

10. "The Radiation Gauge in General Relativity," Phys. Rev., D17, 1945, 1978, with J.W. York, Jr.

11. "Kinematic Conditions in the Construction of Spacetime," Phys. Rev., D17, 2529, 1978, with J.W. York, Jr.

12. "Time Functions in Numerical Relativity: I. Marginally Bound Dust Collapse," Phys. Rev., D19, 2239, 1979, with D. Eardley.

13. "Basic Concepts in Finite Differencing of Partial Differential Equations," p. 139, in Sources of Gravitational Radiation, ed. L. Smarr (Cambridge University Press, 1979).

14. "Gauge Conditions, Radiation Formulae, and the Two Black Hole Collision," p. 245, in Sources of Gravitational Radiation, ed. L. Smarr (Cambridge University Press, 1979).

Professional Articles (continued)

15. "Observations of X-ray Sources in M31," Ap.J.Lett., 234, L45, 1979, with L. Van Speybroeck, A. Epstein, W. Forman, R. Giacconi, C. Jones, and W. Liller.

16. "General Relativistic Hydrodynamics: The Comoving, Eulerian, and Velocity Potential Formalism," Essays in General Relativity: A Festschrift for Abraham Taub (Academic Press 1980), with C. Taubes and J.R. Wilson.

17. "Rayleigh-Taylor Overturn in Supernova Core Collapse," Ap.J., 246, 515, 1981, with J.R. Wilson, R.T. Barton, and R.L. Bowers.

18. "Hydrodynamical Formation of Twin-Exhaust Jets," Ap.J., 247, 52, 1981, with M.L. Norman and J.R. Wilson.

19. "Can the Twin-Exhaust Model Explain Radio Jets?," Nature, 293, 277, 1981, with M.D. Smith, J.R. Wilson and M.L. Norman.

20. "Dumbbell Galaxies and Precessing Radio Jets," Astron.J., 87, 602, 1982, with J.S. Gallagher and A. Wirth.

21. "The Extended Radio Source in the Center of M31," Ap.J.Lett., 257, L13, 1982, with R.M. Hjellming.

22. "Bubbles, Jets and Clouds in Active Galactic Nuclei," Ap.J., 264, 432, 1983, with M.D. Smith, J.R. Wilson, and M.L. Norman.

23. "Structure and Dynamics of Supersonic Jets," Astron. & Astrophys., 113, 285, 1982, with M. Norman, K.-H. Winkler, and M. Smith.

24. "Gravitational Waves and Red Shifts: A Space Experiment for Testing Relativistic Gravity Using Multiple Time-Correlated Radio Signals," Gen. Rel. and Grav., Vol. 15, No. 2, 129, 1983, with R.F.C. Vessot, C.A. Lundquist, R. Decker and T. Piran.

25. "The Missing Bulge Globular Clusters in M31: New Optical Candidates," (submitted August 1982), in press, Ap.J., with A. Wirth and T.L. Bruno.

26. "Black Pits in Cluster Cores," (Univ. of Illinois Astronomy Dept. preprint IAP82-39), submitted to Astronomical Journal, with R. Blandford.

27. "The Contributions of Bryce DeWitt to Classical General Relativity," to appear in Ahead of His Time: Bryce S. DeWitt. Essays on the Quantum Theory of Gravity in Honor of his 60th Birthday, ed. S. Christensen (Adam Hilger, Lmt.: Bristol, England), in press for fall 1983 (Univ. of Illinois Astronomy Dept. preprint IAP83-8).

28. "Propagation and Morphology of Pressure-Confined Supersonic Jets," (Max-Planck Institut für Physik und Astrophysik preprint MPA 61, March 1983), to appear in the Proceedings of the Torino Workshop on Astrophysical Jets, ed. Ferrari and Pacholczyk, with K.-H. Winkler and M. Norman.

Professional Articles (continued)

29. "Numerical Models of Fat Disks: New Scenarios for Fluid Accretion into Black Holes," (Univ. of Illinois Astronomy Dept. preprint IAP83-14), to appear in Numerical Astrophysics: A Meeting in Honor of Jim Wilson, ed. J. Centrella, with J. Hawley.

30. "A Numerical Study of Nonspherical Black Hole Accretion. I. Equations and Test Problems," submitted to Ap.J. May 1983, (Univ. of Illinois Astronomy Dept. preprint IAP83-9), with J. Hawley and J. R. Wilson.

31. "A Numerical Study of Nonspherical Black Hole Accretion. II. Finite Differencing and Code Calibration," (Univ. of Illinois Astronomy Dept. preprint IAP83-13), submitted to Ap.J.Suppl., with J. Hawley and J.R. Wilson.

32. "General Relativistic Magnetohydrodynamics," (Univ. of Illinois Astronomy Dept. preprint IAP83-15), to appear in Numerical Astrophysics: A Festschrift in Honor or James R. Wilson, ed. J. Centrella, with J. Sloan.

Books Published

Sources of Gravitational Radiation, ed. L. Smarr (Cambridge University Press, 1979).

Published Popular Articles or Short Notes

1. "Our Elastic Spacetime: Black Holes and Gravitational Waves," American Scientists, 66, 72, 1978, with W.H. Press.

2. "Black Holes," in Academic American Encyclopedia (Arete, 1979).

3. "Numerical Construction of Spacetime," Proc. R. Soc. Lond., 368, 15 (1979).

4. "Einstein's Impact on the Contemporary World," available from Resident Associate Program, Smithsonian Institution, Washington, D.C., 1979.

5. "Earthport," Future Life, #12, 1979.

6. "Earthport - An International Space Launch Site," Space Age Rev., Mar.-Apr., 1979.

7. "Research Activities of the University of Illinois Department of Astronomy," Bulletin of American Astronomical Society, Vol. 14, No. 1, pp. 209-222, (1982).

8. "Black Hole Accretion: The Quasar Powerhouse," in Energy and Technology Review, March 1983 issue, with J. Hawley.

9. "Some Examples of Supercomputing Projects," in the Report of the Panel on Large Scale Computing in Science and Engineering, P.D. Lax, Chairman (1982).

10. "The Supercomputer Famine in American Universities," in the Report of the Panel on Large Scale Computing in Science and Engineering, P.D. Lax, Chairman (1982).

Papers in Preparation
(i) invited papers - due by Summer 1983

1. "Shock Structures of Pressure Confined Supersonic Jets," to appear in Numerical Astrophysics: A Meeting in Honor of Jim Wilson, ed. J. Centrella, with K.-H. Winkler and M. Norman.

2. "Shocks, Interfaces and Patterns in Supersonic Jets," to appear in Fronts, Interfaces and Patterns, ed. L. Campbell, with K.-H. Winkler and M. Norman.

3. "Timelike Evolution of Einstein's Equations," to appear in Radiation Hydrodynamics, ed. M. Norman and K.-H. Winkler (Reidel, 1983), with J.R. Wilson.

4. "Supersonic Jets," to appear in Radiation Hydrodynamics, ed. M. Norman and K.-H. Winkler (Reidel, 1983), with M. Norman and K.-H. Winkler.

(ii) papers in draft form

6. "The M31 Bulge X-Ray Sources," to be submitted to Ap.J.Lett., with A. Wirth and L. van Speybroeck.

7. "A Numerical Study of Nonspherical Black Hole Accretion. III. Dynamics of Fat Disks Around Black Holes," with J. Hawley and J. R. Wilson.

8. "Hot Spots From Numerical Beam Cap Simulations," to be submitted to Astron. & Astrophys., with M. Smith, M. Norman and K.-H. Winkler.

9. "The Gravitational Potential Well of Galaxy Clusters," with D. Sumi.

Workshops Organized

1. Workshop on Initial Data for Nonspherical Collapse, June 2 - 5, 1975, University of North Carolina (with James York).

2. Princeton Informal Relativity Conference, June 30 - July 2, 1975, Princeton University (with William Press).

3. Workshop on Dynamical Construction of Spacetime, April 19 - 22, 1977, Yale University (with Douglas Eardley and Vincent Moncrief).

4. Symposium on Computer Techniques in General Relativity, August 8, 1977 at Eighth International Conference on General Relativity and Gravitation, Waterloo, Canada.

5. Workshop on Sources of Gravitational Radiation, July 24 - August 4, 1978, Batelle Seattle Research Center, Seattle, Washington.

6. Workshop on Computational Astrophysics, summer 1982, Munich, Germany (with K.-H. Winkler, M. Norman, Dimitri Mihalas).

7. Numerical Astrophysics: A Festschrift for James R. Wilson, Oct. 1982, Univ. of Illinois, Urbana, Ilinois (with J. Centrella and F. Lamb).

8. 10^{th} International Conference on General Relativity and Gravitation Workshop on Numerical Relativity, July 4-9, 1983, Padova, Italy.

Abstracts Published

1. "High Velocity Collision of Two Black Holes -- Initial Data," Bull. Amer. Phys. Soc., 18, 643, 1973, with B. DeWitt.

2. "Collision of Two Black Holes: Computer Generated Spacetime," Bull. Amer. Phys. Soc., 19, 68, 1974, with B. DeWitt.

3. "Minimal Shear and Maximal Slices," Bull. Amer. Phys. Soc., 20, 544, 1975, with J. York.

4. "Collision of Two Black Holes: Stabilizing the Constraints," Bull. Amer. Phys. Soc., 20, 544, 1975, with K. Eppley.

5. "Possible Companions of the Taylor-Hulse Pulsar," Bull. Amer. Phys. Soc., 20, 632, 1975, with R. Blandford and J.P. Ostriker.

6. "Tidal Circularization Induced in Close Binaries by Turbulent Viscosity," Bull. Amer. Astron. Soc., 7, 534, 1975, with W.H. Press and P. Wiita.

7. "Gravitational Wave Generation Efficiency for Colliding Black Holes," Bull. Amer. Astron. Soc., 8, 516, 1976.

8. "Colliding Black Holes," GR8 Abstracts of Contributed Paper, p. 18, 1977.

9. "Nonspherical Gravitational Collapse," Bull. Amer. Astron. Soc., 10, 656, 1978.

10. "Numerical Simulation of Fat Disks Around Black Holes," Bull. Amer. Astron. Soc., 14, 869, 1982, with J. Hawley and J.R. Wilson.

11. "Wide-Angle-Tail Radio Sources, X-ray Cooling Cores, and Black Pits," Bull. Amer. Astron. Soc., 14, 870, 1982, with D. Sumi.

Courses Taught

1. "The Interstellar Medium," Senior Level Undergraduate Semester Course, Department of Astrophysical Sciences, Princeton University, Spring, 1975.

2. "Thought and Structure in Physical Science," Undergraduate Semester Course, Department of Astronomy, University of Illinois, Fall 1979 and 1980.

3. "General Relativity," Graduate Semester Course, Department of Physics and Astronomy, University of Illinois, Fall, 1981.

4. "Descriptive Astronomy," Undergraduate Semester Course, Department of Astronomy, University of Illinois, Spring 1982 and Fall 1982.

5. "The Physical Universe," Undergraduate Semester Course, Department of Astronomy, University of Illinois, Spring 1980, 1981 and 1983.

Letters of Recommendation

Dr. Bryce DeWitt -- Physics Department, University of Texas

Dr. Ron Ekers -- Director, VLA

Dr. William Press -- Chairman, Astronomy Department, Harvard University

Dr. Kip Thorne -- California Institute of Technology

Dr. James R. Wilson -- Lawrence Livermore Laboratory

Dr. Kenneth Wilson -- Cornell University

JOHN B. KOGUT

Present position: Professor of Physics
Date of Birth: March 6, 1945

Education: B. A. Princeton University, 1967
M. S. Stanford University, 1968
Ph.D. Stanford University, 1971

Scientific Experience:

Research Associate, Institute for Advanced Study,
Princeton, September 1971 - April 1973
Visiting Research Associate, Tel Aviv University, April - August 1973
Research Associate, Cornell University, Fall 1973
Assistant Professor, Cornell University, Fall 1974-1978
Professor, University of Illinois, Fall 1978 to present

Awards, Grants, National Committees:

Sloan Foundation Fellow, 1976-1978
Fellow in the American Physics Society (elected, 1983)
High Energy Theory Grant, NSF PHY82-01948
Served on T.A.C.U.P. Review Panal of the Department of Energy (1983)
Listed in American Men and Women in Science and Technology and in Who's Who in American Technology.

Publications:

Production of Strongly Interacting W's in Inelastic Electron-Nucleon Collisions. Phys. Rev. 186, 1540 (1969).

With D. E. Soper. Quantum Electrodynamics in the Infinite Momentum Frame. Phys. Rev. D1, 2901 (1970).

Quantum Electrodynamics at Infinite Momentum: Applications to High Energy Scattering (Thesis) SLAC Report 138, (1971).

With J. D. Bjorken and D. E. Soper. Quantum Electrodynamics at Infinite Momentum: Scattering from and External Field. Phys. Rev. D3, 1382 (1971).

Role of Interacting Reggeons in Field-Theoretic Investigations of High Energy Scattering. Phys. Rev. D4, 3101 (1971).

With S. M,. Berman and J. D. Bjorken. Inclusive Processes at High Transverse Momentum. Phys. Rev. D4, 3388 (1971).

Pion Condensation and Properties of Neutron Stars. Invited talk to the Sixth Texas Symposium on Relativistic Astrophysics, December 1972. Annals of the New York Academy of Sciences 224, p. 266.

Electroproduction and the "Size" of a Virtual Photon. Phys. Rev. D5, 1152 (1972).

Publications continued - John Kogut

With H. D. I. Abarbanel. Effect of Virtual Photon Mass on Transverse Momentum Distributions in Inclusive Processes. Phys. Rev. D5, 2050 (1972).

With G. Frye and L. Susskind. Hard and Soft Processes in Hadrodynamics. Phys. Letters 40B, 469 (1972).

With J. Manassah. Pion Condensation and Neutron Star Cooling. Phys. Letters 41A, 129 (1972).

Recent Advances in Theories of Deep Inelastic Phenomena. Invited talk at the August 1973 Berkeley meeting of the Division of Particles and Fields of the American Physical Society. AIP Conference Proceedings, Particles and Fields -- 1973, p. 102 - 120.

With L. Susskind. Everything You Always Wanted to Know about Partons, But Were Afraid to Ask. Physics Reports 8C, 75 (1973).

With D. K. Sinclair and L. Susskind. Hadronic Final States of Deep Inelastic Processes in Simple Quark Parton Models. Phys. Rev. D7, 3637 (1973).

With J. D. Bjorken. Correspondence Arguments for High Energy Scattering. Phys. Rev. D8, 1341 (1973).

Resonance and Parton Model Descriptions of Final States of Deeply Inelastic Reactions. Phys. Rev. D8, 3029 (1973).

With A. Casher and L. Susskind. Theory of Non-Strange Currents and Mesons. Phys. Rev. D8, 4448 (1973).

With A. Casher and L. Susskind. Vacuum Polarization and the Quark-Parton Puzzle. Phys. Rev. Lett. 31, 792 (1973).

Problems and Progress in Constituent Theories of Hadrons. Invited talk at the September 1974 Williamsburg meeting of the Division of Particles and Fields of the American Physical Society. AIP Conference Proceedings, Particles and Fields -- 1974, p. 458-481.

With L. Susskind. The Scale Invariant Parton Model. Phys. Rev. D9, 697 (1974).

With A. Casher and L. Susskind. Consequences of the Scale Invariant Parton Model for Deep Inelastic Neutrino Scattering. Phys. Rev. D9, 706 (1974).

With L. Susskind. Parton Models and Asymptotic Freedom. Phys. Rev. D9, 3391 (1974).

With A. Casher and L. Susskind. Vacuum Polarization and the Absence of Free Quarks. Phys. Rev. D10, 732 (1974).

With D. K. Sinclair. (1+1)-Dimensional Models of Quark Confinement and Final States in Deep-Inelastic Scattering. Phys. Rev. D10, 4181 (1974).

Publications continued - John Kogut

With L. Susskind. Vacuum Polarization and the Absence of Free Quarks in Four Dimensions. Phys. Rev. D9, 3501 (1974).

With L. Susskind. Quark Confinement and the Puzzle of the Ninth Axial-Vector Current. Phys. Rev. D10, 3468 (1974).

Electron-Positron Annihilation and Speculations on the Renormalization Group of Strong Interactions. Phys. Lett. B51, 383 (1974).

With K. G. Wilson. The Renormalization Group and the ε-Expansion. Physics Reports 12C, 75 (1975).

With L. Susskind. How Quark Confinement Solves the $\eta \to 3\pi$ Problem. Phys. Rev. D11, 3594 (1975).

With R. F. Cahalan, K. A. Geer and L. Susskind. Asymptotic Freedom and the "Absence" of Vector-Gluon Exchange in Wide-Angle Hadronic Collisions. Phys. Rev. D11, 1199 (1975).

With L. Susskind. Hamiltonian Formulation of Wilson's Lattice Gauge Theory. Phys. Rev. D11, 395 (1975).

With E. Eichten, K. Gottfried, T. Kinoshita, K. D. Lane and T.-M. Yan. The Spectrum of Charmed Quark-Antiquark Bound States. Phys. Rev. Lett. 34, 369 (1975).

With L. Susskind. Electron-Positron Annihilation At and Above the Threshold for Production of Charmed Hadrons. Phys. Rev. Lett. 34, 767 (1975).

With L. Susskind. Electron-Positron Annihilation Cross Section Near the New Threshold. Phys. Rev. D12, 2821 (1975).

With D. K. Sinclair. Quark Confinement and the Evasion of Goldstone's Theorem in 1+1 Dimensions. Phys. Rev. D12, 1742 (1975).

With T. Banks and L. Susskind. Strong Coupling Calculations of Lattice Gauge Theories: 1+1 Dimensional Exercises. Phys. Rev. D13, 1043 (1976).

With L. Susskind. New Ideas about Confinement. Reprinted in "Extended Systems in Field Theory", Physics Reports 23C, 237 (1976).

With A. Carroll, D. K. Sinclair and L. Susskind. Lattice Gauge Theory Calculations in 1+1 Dimensions and the Approach to the Continuum Limit. Phys. Rev. D13, 2270 (1976).

With D. K. Sinclair and L. Susskind. A Quantitative Approach to Low-Energy Quantum Chromodynamics. Nucl. Phys. B114, 199 (1976).

Massive μ-pair Production in Hadron-Hadron Collisions and the Asymtotically Free Parton Model. Phys. Lett. 65B, 377 (1976).

Publications continued - John Kogut

Three Lectures on Lattice Gauge Theory presented at the International Summer School, McGill University, June 21-26, 1976. Reprinted in the Proceedings of the Summer School.

Three Lectures on Lattice Gauge Theory Presented at the International Summer Institute for Theoretical Physics, University of Bielefeld, August 23 - Sept. 4, 1976. Reprinted in the Proceedings of the Conference.

With T. Banks, S. Raby, L. Susskind, D. R. T. Jones, P. N. Scharbach and D. K. Sinclair. Strong-Coupling Calculations of the Hadron Spectrum of Quantum Chromodynamics. Phys. Rev. D15, 1111 (1977).

With J. Shigemitsu. Comparison of Recent Massive Muon Data with the Asymptotically Free Parton Model. Physics Letters 71B, 165 (1977).

With J. Shigemitsu. Estimates for W^{+}, Z° and μ-pair Production in the Asymptotically Free Parton Model. Nucl. Phys. B129, 461 (1977).

With T. Banks and R. Myerson. Phase Transitions in Abelian Lattice Gauge Theories. Nucl. Phys. B129, 493 (1977).

With D. R. T. Jones, P. N. Scharbach and D. K. Sinclair. Lattice Gauge Theory Calculations of f_{π} and f_{ρ}. Phys. Rev. D17, 1871 (1978).

"A Review of Developments in Lattice Gauge Theory: Extreme Environments and Duality Transformations", presented at the conference, "Current Trends in the Theory of Fields", Florida State University, April 6-7, 1978.

With C. J. Hamer and L. Susskind. Phases of Two Dimensional Heisenberg Spin Systems from Strong Coupling Expansions. Phys. Rev. Lett. 41, 1337 (1978).

With W. Fischler and L. Susskind. Quark Confinement in Unusual Environments. Phys. Rev. D19, 1188 (1979).

With C. J. Hamer and L. Susskind. Strong Coupling Expansions of Phase Diagrams for the O(2), O(3) and O(4) Heisenberg Spin Systems in Two Dimensions. Phys. Rev. D19, 3091 (1979).

With D. K. Sinclair and D. R. T. Jones. The Electrodynamics of the Planar Model: Its Phase Diagram, Continuum Limit, and Mass Spectrum. Phys. Rev. D19, 1882 (1979).

With A. Carroll. Improved Strong-Coupling Expansions and Matrix Pade Approximants for Lattice Theories. Phys. Rev. D19, 2429, (1979).

With D. R. T. Jones, R. D. Kenway and D. K. Sinclair. Lattice Gauge Theory Calculations Using an Improved Strong-Coupling Expansion and Matrix Pade Approximants. Nucl. Phys. B158, 102, (1979).

Publications continued - John Kogut

With D. R. T. Jones and D. K. Sinclair. Effective Hamiltonians and Degenerate Perturbation Theory Calculations of the Mass Spectrum in Lattice Q.C.D. Zeitschrift für Physik C3, 29, (1979).

With C. J. Hamer. Accurate Results from Hamiltonian Strong-Coupling Expansions of the Ising, Planar, O(3) and O(4) Spin Systems. Phys. Rev. B20, 3859, (1979).

With R. B. Pearson and J. Shigemitsu. Quantum Chromodynamic β Function at Intermediate and Strong Coupling. Phys. Rev. Lett. 43, 484, (1979).

An Introduction to Lattice Gauge Theory and Spin Systems. Rev. Mod. Phys. 51, 659, (1979).

1/N Expansions and the Phase Diagram of Discrete Lattice Gauge Theories with Matter Fields. Phys. Rev. D21, 2316, (1980).

With R. B. Pearson and J. Shigemitsu. The String Tension Confinement and Roughening in SU(3) Hamiltonian Lattice Gauge Theory. Phys. Lett. 98B, 63, (1980).

With J. Shigemitsu. Crossover from Weak to Strong Coupling in SU(N) Lattice Gauge Theories. Phys. Rev. Lett. 44, 410, (1980).

With R. B. Pearson and J. Shigemitsu. Hamiltonian Potts Models. Institute for Theoretical Physics, Santa Barbara Internal Report (1980).

With C. J. Hamer. Weak Coupling Series and the Critical Indices of Z_N Spin Systems in Two Dimensions. Phys. Rev. B22, 3378, (1980).

With R. B. Pearson, J. Shigemitsu and D. K. Sinclair. Z_n and N-state Potts Lattice Gauge Theories: Phase Diagrams, First Order Transitions, Functions and 1/N Expansions. Phys. Rev. D22, 2447, (1980).

With D. K. Sinclair. 1/Q Expansions and the First Orders Phase Transitions of the Three-State Potts Model in 3 Dimensions. Phys. Lett. 81A, 149, (1981).

With D. K. Sinclair. More on Potts Lattice Gauge Theories. Phys. Rev. D23, 2967 (1981).

With J. Shigemitsu and D. K. Sinclair. Comparing O(N) and SU(N) x SU(N) Spin Systems in 1+1 Dimensions to SU(N) Gauge Theories in 3+1 Dimensions. Phys. Lett. 100B, 316 (1981).

With D. K. Sinclair, R. B. Pearson, J. L. Richardson and J. Shigemitsu. The Fluctuating String of Lattice Gauge Theory: The Heavy Quark Potential, Restoration of Rotational Symmetry and Roughening. Phys. Rev. D23, 2945, (1981).

Publications continued - John Kogut

With D. K. Sinclair. On the Analyticity of the Off-Axis String Tension and the Restoration of Rotational Symmetry in Lattice Systems. Phys. Rev. D24, 1610 (1981).

With J. Shigemitsu. A Study of Λ Parameters and Crossover Phenomena in SU(N) x SU(N) Sigma Models in Two Dimensions. Nucl. Phys. B190, 365, (1981).

Publications continued - John Kogut

With D. K. Sinclair. 1/Q Expansions for Potts Models in All Dimensions. Phys. Lett. 86A, 38 (1981).

With G. Parisi. Long Range Spin-Spin Forces in Gauge Theories. Phys. Rev. Lett. 47, 1089 (1981).

With M. Snow, and M. Stone. Computer Simulations of SU(N) X SU(N) Spin Systems in Two Dimensions. Phys. Rev. Lett. 47, 1767 (1981).

With M. Snow and M. Stone. Mean Field and Monte Carlo Studies of SU(N) Chiral Models in Three Dimensions. Nucl. Phys. B200 [FS4], 211 (1982).

With C. J. Hamer, D. P. Crewther, M. M. Mazzolini. The Massive Schwinger Model on a Lattice: Background Field, Chiral Symmetry, and the String Tension. Nucl. Phys. B208, 413 (1982).

With M. Stone, H. W. Wyld, J. Shigemitsu, S. H. Shenker and D. K. Sinclair. Scales of Chiral Symmetry Breaking in Quantum Chromodynamics. Phys. Rev. Lett. 48, 1140 (1982).

With D. K. Sinclair. 1/Q Expansions for the Lagrangian Formulation of Three Dimensional Potts Models. Solid State Commun. 41, 187 (1982).

A Review of the Lattice Gauge Theory Approach to Quantum Chromodynamics. Invited lectures at the 1982 Les Houches and St. Andrews Summer Schools in Theoretical Physics. To appear in Rev. Mod. Phys., July, 1983.

With J. Carlson and V. R. Pandharipande. A Quark Model for Baryons based on Quantum Chromodynamics, Phys. Rev. D27, 233 (1983).

With M. Stone and M. Snow. SU(N) x SU(N) Spin Systems in Two Dimensions Crossover, Variant Actions and Finite Size Scaling. Nucl. Phys. B215, 45 (1983).

With W. R. Gibbs, S. H. Shenker, J. Shigemitsu, D. K. Sinclair, M. Stone and H. W. Wyld. Deconfinement and Chiral Symmetry Restoration at Finite Temperatures in SU(2) and SU(3) Gauge Theories, Phys. Rev. Lett. 50, 393 (1983).

With H. Matsuoka, S. H. Shenker, J. Shigemitsu, D. K. Sinclair, M. Stone and H. W. Wyld. Quark and Gluon Latent Heats at the Deconfinement Phase Transition in SU(3) Gauge Theory. Illinois Theoretical Physics Preprint 83-9, April 1983 (submitted to Phys. Rev. Lett.).

Publications continued - John Kogut

With H. Matsuoka, S. H. Shenker, J. Shigemitsu, D. K. Sinclair, M. Stone and H. W. Wyld. Chiral Symmetry Restoration in Baryon Rich Environments. Illinois Theoretical Physics Preprint 83-10, April 1983 (to appear in Nucl. Phys.).

With S. H. Shenker, J. Shigemitsu, D. K. Sinclair, M. Stone and H. W. Wyld. Studies of Chiral Symmetry Breaking in SU(2) Gauge Theory. Ohio State University Theoretical Physics Preprint, DOE/ER/01545-335 (submitted to Nucl. Phys).

With J. Carlson and V. R. Pandharipande. Hadron Spectroscopy in a Flux-Tube Quark Model. Illinois Nuclear Physics Preprint 83-18, June 1983 (submitted to Phys. Rev. D.).

Current NSF Grants:

NSF-PHY82-01948 "Theoretical Physics and Nuclear Physics"
Principals: D.G. Ravenhall and H. W. Wyld
Additional Faculty: J. B. Kogut, S. J. Chang, J. D. Sullivan
Acct.# 1-5-29234
Duration: 5 Years (Beginning 1982)

NSF-PHY83-04872 "Upgrade the Central Memory of An Array Processor Attached to a VAX Network"
Principals: J. B. Kogut, J. D. Stack, H. W. Wyld
Status: Proposed beginning date: Fall, 1983. (Formal authorization pending)

Professional Resume -- David J. Kuck

Born: October 3, 1937, Muskegon, Michigan

Education: B.S.E.E., University of Michigan, 1959
M.S. , Northwestern University, 1960
Ph.D. , Northwestern University, 1963

Employment:

1963-1965: Ford Postdoctoral Fellow and Assistant Professor of Electrical Engineering, MIT, Cambridge, MA.
Research at Project MAC on time-sharing and formal languages.
Teaching of software and language courses.

1965--present: Department of Computer Science, University of Illinois, Urbana.
1965-1968, Assistant Professor; 1968-1972, Associate Professor; presently, Professor.

Research:

1969--present: Study of various machine and software organization problems. These include parallel, pipeline, and multiprocessor computation methods, interconnection networks, memory hierarchies, and the compilation of ordinary programs for such machines. Theoretical as well as empirical studies are being carried out.

Also, we are investigating certain classes of file processing and information retrieval problems to achieve high system performance. This involves the organization of very large data-bases, their storage in a memory hierarchy, and access algorithms. Architectures for high-speed processing of such data are being considered.

Memberships:

1982-1983: Associate Member, Center for Advanced Studies, University of Illinois at Urbana-Champaign.

1983: Senior Member, The Institute of Electrical and Electronics Engineers, Inc. (IEEE)

Some Recent Invited Lectures:

1979	Munich, Germany, Siemens Seminar on New Computer Architectures
1980	Shanghai and Peking, China; Fudan and Tsinghua Universities
1980	Loughborough University of Technology, Loughborough, England; CREST Parallel Processing Systems Course
1981	Bergamo, Italy, University of Bergamo, CREST Conference on Design of Numerical Algorithms for Parallel Processing
1981	Nurnberg, F. R. Germany, CONPAR 81, Conference on Analysing Problem-Classes and Programming for Parallel Computing
1981	Minneapolis, MN, University of Minnesota, Distinguished Lecturer
1982	Seattle, WA, University of Washington, Distinguished Lecturer
1982	Paris, France, University of Paris and INRIA
1983	Los Alamos, NM, Los Alamos National Laboratory, Frontiers of Supercomputing
1983	Norfolk, VA, Fall SIAM Meeting

Consulting Activities:

1968-1969:	Standard Oil of Indiana Corporate Headquarters, Chicago, IL Corporate long-range data processing planning
1971:	RAND Corporation Computer Science Group, Santa Monica, CA Studies of computer systems
1971-1972:	NASA Ames Research Center, Moffett Field, CA ILLIAC IV software and system studies
1972-1980:	Burroughs Corporation, Paoli, PA, Advanced Development Organization. Studies of high-speed computation, principal architect of Burroughs BSP system
1971-1973:	U. S. Army Computer Systems Command (SAMAC), Ft. Belvoir, VA Army computer systems and management
1974:	National Bureau of Standards, Washington, DC Computer capacity and performance studies
1977-1979:	National Science Foundation, Washington, DC Advisory Panel on Computer Science
1978--present:	Los Alamos Scientific Laboratory, Los Alamos, NM Parallel algorithms and computer architecture

1978-1979: National Science Foundation, Washington, DC
Advisory Panel, Integrated Basic Research Division

1978-1979: Univac, Roseville, MN
Software and architecture for high-speed computation

1979--present: Kuck and Associates, Inc., Champaign, IL
Computer architecture, design automation, and compilers for pipeline, parallel, and multiprocessor systems

1980--present: Birkhauser Boston, Inc., Cambridge, MA
Publishing Consultation

Other Professional Activities:

1973: U. S. Delegate to Popov Society Congress, Moscow

1973-1975: Associate Editor for Computer Architecture and Systems, IEEE Transactions on Computers

1973-1974: Institute for Electronics and Electrical Engineers (IEEE) Computer Society Distinguished Visitor

1973-1974: Association for Computing Machinery (ACM) Lecturer

1977-1981: Associate Editor, ACM Transactions on Database Systems

1977--present: Associate Editor, International Journal of Computer and Information Sciences

1977: Chairman, Symposium on High Speed Computer and Algorithm Organization

1980--present: Area Editor, for Computer Organization and Design, Journal of the ACM

1980--present: Associate Editor, Journal of Digital Systems

1982: Editorial Board, Computer Engineering

Program Committees:

1975	ACM SIGPLAN Array Languages
1979	Texas Conference on Computing
1980	Co-Chairman, International Conference on Parallel Processing
1980	ACM SIGMOD Conference
1980	The 7th International Symposium on Computer Architecture
1981	The 8th International Symposium on Computer Architecture
1981	IEEE COMPCON 81 Fall Computer Conference
1983	10th International Symposium on Computer Architecture
1983	NATO Advanced Study Institute (Chairman)
1983	Conference on Potential of Parallel Processing for Scientific Computing (SIAM)
1983	Parallel Computing '83 (Berlin)

Current Research Grants:

National Science Foundation April 1, 1980--September 30, 1983
"Computer System Organization"

National Science Foundation May 1, 1981--April 30, 1984
"Software Studies for Parallel Memories, Multiprocessors, and Virtual Memories"

U. S. Department of Energy January 1, 1981--December 31, 1983
"Design, Evaluation and Use of High Performance Computer Systems"

Control Data Corporation March 1, 1982--February 29, 1984
"Parafrase System Research"

BOOKS AND BOOK CHAPTERS

	FILE NO.	TITLE	AUTHOR(S)
1970	10	"The Use and Performance of Memory Hierarchies: A Survey," Software Engineering, Vol. 1, Academic Press, Inc., NY and London, 1970. (Julius T. Tou, Ed.)	D. J. Kuck and D. H. Lawrie
	8	Investigation of New Technical Developments in Electronic Computers, published by Japanese Electronic Industry Development Association, No. 45-C-205, Tokyo, Japan, Mar. 1970.	D. J. Kuck
1973	61	"Multioperation Machine Computational Complexity," in Complexity of Sequential and Parallel Numerical Algorithms, pp. 17-47, Ed. by J. F. Traub, Academic Press, 1973.	D. J. Kuck
1974	40a	"Implementation and Considerations for Masking Rotational Latency by Dynamic Disk Allocation," in Computer Architectures and Networks, pp. 207-237. Ed. by E. Gelenbe and R. Mahl. (Amsterdam: North-Holland Publ. Co., 1974)	D. E. Gold and D. J. Kuck
1976	127	"Parallel Processing of Ordinary Programs," in Advances in Computers, Vol. 15, pp. 119-179. Ed. by M. Rubinoff and M. C. Yovits (Academic Press, 1976).	D. J. Kuck
	70	"Supercomputers, Implementations," in Encyclopedia of Computer Science, First Edition, pp. 1376-1382. Ed. by A. Ralston and C. L. Meek (NY: Petrocelli/Charter, 1976).	D. J. Kuck and D. H. Lawrie
	71	"Supercomputers, Principles," in Encyclopedia of Computer Science, First Edition, pp. 1373-1376. Ed. by A. Ralston and C. L. Meek (NY: Petrocelli/Charter, 1976).	D. J. Kuck
1977	182	High Speed Computer and Algorithm Organization, Academic Press, Inc., NY, 1977.	D. J. Kuck, D. H Lawrie and A. H. Sameh (Editors)
1978	178	The Structure of Computers and Computations, Vol. I, John Wiley & Sons, Inc., NY, 1978.	D. J. Kuck
1982	247	"Supercomputer Principles," in Encyclopedia of Computer Science, Second Edition, ed. by A. Ralston, pp. 1455-1458, (NY: Van Nostrand Reinhold Co.), 1982.	D. J. Kuck
	248	"Pipelining Techniques and Array Processors," in Encyclopedia of Computer Science, Second Edition, ed. by A. Ralston, pp. 1143-1145 (NY: Van Nostrand Reinhold Co.), 1982.	D. J. Kuck and D. D. Gajski

CONFERENCE PROCEEDINGS

	FILE NO.	TITLE	AUTHOR(S)
1969	14	"TRANQUIL: A Language for an Array Processing Computer," Joint Computer Conference, AFIPS Proc., Vol. 34, AFIP Press, Montvale, NJ, pp. 57-73, 1969.	Norma E. Abel, Paul P. Budnik, David J. Kuck, Yoichi Muraoka, Robert S. Northcote and Robert B. Wilhelmson
1972	11	"Parallel Computation of Eigenvalues of Real Matrices," in Information Processing 71, Vol. II, pp. 1266-1272, North-Holland Publ. Co., Amsterdam-London, 1972.	D. J. Kuck and Ahmed H. Sameh
	24	"Interconnection Networks for Processors and Memories in Large Systems," Compcon 72, IEEE Computer Society Conference Proceedings, pp. 131-134, Sept. 1972.	D. J. Kuck, D. H. Lawrie and Y. Muraoka
	23	"Fast Computers from Slow Parts," Compcon 72, IEEE Computer Society Conf. Proceedings, pp. 49-52, Sept. 1972.	D. J. Kuck and Y. Muraoka
	30	"Supercomputers for Ordinary Users," Proceedings of the 1972 Fall Joint Computer Conference, Vol. 41, Part I, pp. 213-220, 1972.	David J. Kuck
1973	62	"Multioperation Machine Processing of Ordinary Programs," Invited paper, Proceedings of the First International Symposium on Computers and Chinese Input/Output Systems, pp. 653-672, Aug. 1973.	D. J. Kuck
1975	119	"ROM-Rounding: A New Rounding Scheme," Proc. of the Third IEEE Symposium on Computer Arithmetic, pp. 67-72, Nov. 1975.	D. J. Kuck, D. S. Parker, Jr. and A. H. Sameh
1976	96	"On the Speedup and Cost of Parallel Computation," in The Complexity of Computational Problem Solving, R. S. Anderssen and R. P. Brent, eds., University of Queensland Press, St. Lucia, Queensland, pp. 63-78, 1976.	D. J. Kuck
	122	"The Design of System Architectures for Information Retrieval," Proc. of the ACM 76 National Conference, Aug. 1976.	L. A. Hollaar, B. J. Hurley, D. J. Kuck, D. H. Lawrie, J. W. S. Liu, J. M. Milner, J. K. Morgan, J. R. Rinewalt and W. H. Stellhorn

CONFERENCE PROCEEDINGS (Cont'd.)

	FILE NO.	TITLE	AUTHOR(S)
1976	133	"A System Model for Computer Performance Evaluation," Proc. of the International Symposium on Computer Performance Modeling, Measurement and Evaluation, pp. 187-199, Mar. 1976.	D. J. Kuck and B. Kumar
1979	195	"Automatic Program Transformations for Virtual Memory Computers," Proc. of the 1979 National Computer Conf., pp. 969-974, June 1979.	W. Abu-Sufah, D. Kuck and D. Lawrie
	219	"High Speed Multiprocessors and Their Compilers," Proc. of the International Conf. on Parallel Processing, pp. 5-16, Aug. 1979.	D. J. Kuck and D. Padua-Haiek
1980	237	"Automatic Design with Dependence Graphs," Proc. of the 17th Design Automation Conf., Minneapolis, MN, pp. 506-515, June 1980.	A. E. Casavant, D. D. Gajski an D. J. Kuck
	224	"Array Machine Control Units for Loops Containing IFs," Proc. of the 1980 Int'l. Conf. on Parallel Processing; Harbor Springs, MI, pp. 28-36, Aug. 1980.	U. Banerjee, D. Gajski and D. Kuck
	264	"High-Speed Machines and Their Compilers," Proc. of the CREST Parallel Processing Systems Course, D. J. Evans, Ed., Sept. 1980 (Cambridge University Press).	David J. Kuck
	250	"The Structure of an Advanced Vectorizer for Pipelined Processors," Proc. of COMPSAC 80, The 4th Int'l. Computer Software and Applications Conf., Chicago, IL, pp. 709-715, Oct. 1980.	D. J. Kuck, R. H. Kuhn, B. Leasure and M. Wolfe
1981	253	"Dependence Graphs and Compiler Optimizations," Proc. of the 8th ACM Symp. on Principles of Programming Languages (POPL), Williamsburg, VA, pp. 207-218, Jan. 1981.	D. J. Kuck, R. H. Kuhn, D. A. Padua, B. Leasure and M. Wolfe
	254	"Dependence Driven Computation," Proc. of the COMPCON 81 Spring Computer Conf., San Francisco, CA, pp. 168-172, Feb. 1981.	D. D. Gajski, D. J. Kuck and D. A. Padua
	277	"Automatic Program Restructuring for High-Speed Computation," Invited paper, Proc. of CONPAR 81, Conf. on Analysing Problem-Classes and Programming for Parallel Computing, Nurnberg, F. R. Germany, pp. 66-84, June 1981. (Springer-Verlag)	D. J. Kuck
	296	"Languages and Compilers for Parallel and Pipeline Machines," Invited paper, Proc. of the CREST Conf. on Design of Numerical Algorithms for Parallel Processing, Univ. of Bergamo, Bergamo, Italy, June 1981.	D. J. Kuck

CONFERENCE PROCEEDINGS (Cont'd.)

	FILE NO.	TITLE	AUTHOR(S)
1981	297	"Languages and High-Performance Computations," Invited paper, Proc. of the IFIP Working Conf. on The Relationship Between Numerical Computation and Programming Languages, Boulder, CO, ed. by J. Reid, pp. 205-221, Aug. 1982 (North-Holland).	D. Kuck, D. Padua, A. Sameh, & M. Wolfe
	379	"Sparse Structures Taxonomy," to appear in Proc. of the NATO Advanced Research Workshop on High-Speed Computation, Julich, F. R. Germany, ed. by J. S. Kowalik, June 20-22, 1983 (Springer-Verlag). (MCS80-01561, DOE DE AC02-81ER10822, & CDC82-1101)	D. J. Kuck & D. D. Gajski
	354	"CEDAR--A Large Scale Multiprocessor," to appear in Proc. of the 1983 Int'l. Conf. on Parallel Processing, Aug. 1983. (MCS81-00512, MCS80-01561, & US DOE DE-AC02-81ER10822)	Daniel Gajski, David Kuck, Duncan Lawrie & Ahmed Sameh

REFEREED JOURNALS

	FILE NO.	TITLE	AUTHOR(S)
1968	7	"ILLIAC IV Software and Application Programming," IEEE Transactions on Computers, Vol. C-17, No. 8, pp. 758-770, Aug. 1968.	D. J. Kuck
	12	"The ILLIAC IV Computer," IEEE Transactions on Computers, Vol. C-17, No. 8, pp. 746-757, Aug. 1968.	G. Barnes, R. Brown, M. Kato, D. Kuc D. Slotnick and R. Stokes
1969	13	"Seismic Signal Processing via the ILLIAC IV Computer," IEEE Trans. Geoscience Electronics, Vol. GE-7, pp. 34-41, Jan. 1969.	G. M. Ackins an D. J. Kuck
1970	9	"A Preprocessing High-Speed Memory System," IEEE Transactions on Computers, Vol. C-19, pp. 793-802, Sept. 1970.	D. J. Kuck
1971	15	"The Organization and Use of Parallel Memories," IEEE Transactions on Computers, Vol. C-20, pp. 1566-1569, Dec. 1971.	Paul Budnik and David J. Kuck
1972	18	"On the Number of Operations Simultaneously Executable in FORTRAN-Like Programs and Their Resulting Speed-Up," IEEE Trans. on Computers, Vol. C-21, No. 12, pp. 1293-1310, Dec. 1972.	D. J. Kuck, Y. Muraoka and S. C. Chen
1973	19	"On the Time Required for a Sequence of Matrix Products," Communications of the ACM, Vol. 16, pp. 22-26, Jan. 1973.	Yoichi Muraoka David J. Kuck
	22	"The Parallel Evaluation of Arithmetic Expressions Without Division," IEEE Transactions on Computers, Vol. C-22, No. 5, pp. 532-534, May 1973.	Richard Brent, David Kuck and Kiyoshi Maruyam
1974	58	"Bounds on the Parallel Evaluation of Arithmetic Expressions Using Associativity and Commutativity," Acta Informatica, Vol. 3, Fasc. 3, pp. 203-216, 1974.	David Kuck and Yoichi Muraoka
	56	"Measurements of Parallelism in Ordinary FORTRAN Programs," IEEE Computer, Vol. 7, No. 1, pp. 37-46, Jan. 1974.	D. Kuck, P. Budnik, S-C. Chen, E. Davis, Jr., J. Han, P. Kraska, D. Lawrie, Y. Muraoka, R. Strebendt and R. Towle

REFEREED JOURNALS (Cont'd.)

	FILE NO.	TITLE	AUTHOR(S)
1974	40	"A Model for Masking Rotational Latency by Dynamic Disk Allocation," Communications of the ACM, Vol. 17, pp. 278-288, May 1974.	D. E. Gold and D. J. Kuck
1975	69	"Time Bounds on the Parallel Evaluation of Arithmetic Expressions," SIAM Journal of Computing, Vol. 4, No. 2, pp. 147-162, June 1975.	D. J. Kuck and K. Maruyama
	73	"Time and Parallel Processor Bounds for Linear Recurrence Systems," IEEE Trans. on Computers, Vol. C-24, No. 7, pp. 701-717, July 1975.	S. C. Chen and D. J. Kuck
1976	109	"Parallel Poisson and Biharmonic Solvers," Computing, Vol. 17, pp. 219-230, 1976.	A. H. Sameh, S. C. Chen and D. J. Kuck
1977	92	"A Parallel QR Algorithm for Symmetric Tridiagonal Matrices," IEEE Trans. on Computers, Vol. C-26, No. 2, pp. 147-153, Feb. 1977.	A. H. Sameh and D. J. Kuck
	116	"On the Effective Bandwidth of Parallel Memories," IEEE Trans. on Computers, Vol. C-26, No. 5, pp. 480-490, May 1977.	D. Chang, D. J. Kuck and D. Lawrie
	118	"Combinational Circuit Synthesis with Time and Component Bounds," IEEE Trans. on Computers, Vol. C-26, No. 8, pp. 712-726, Aug. 1977.	S. C. Chen and D. J. Kuck
	155	"A Survey of Parallel Machine Organization and Programming," ACM Computing Surveys, Vol. 9, No. 1, pp. 29-59, Mar. 1977.	D. J. Kuck
	157	"Analysis of Rounding Methods in Floating-Point Arithmetic," IEEE Trans. on Computers, Vol. C-26, No. 7, pp. 643-650, July 1977.	D. J. Kuck, D. S. Parker and A. H. Sameh
	158	"Parallel Direct Linear System Solvers--A Survey," Invited paper, Parallel Computers--Parallel Mathematics, Munich, Germany, pp. 25-30, Mar. 1977, North-Holland Publ. Co.; also, Mathematics and Computers in Simulation, Vol. XIX, pp. 272-277, North-Holland Publ. Co., 1977.	A. H. Sameh and D. J. Kuck
1978	137	"On Stable Parallel Linear System Solvers," Journal of the ACM, Vol. 25, No. 1, pp. 81-91, Jan. 1978.	A. H. Sameh and D. J. Kuck
	148	"Practical Parallel Band Triangular System Solvers," ACM Trans. on Mathematical Software, Vol. 4, No. 3, pp. 270-277, Sept. 1978.	S. C. Chen, D. J. Kuck and A. H. Sameh

REFEREED JOURNALS (Cont'd.)

	FILE NO.	TITLE	AUTHOR(S)
1979	105	"Time and Parallel Processor Bounds for Fortran-like Loops," IEEE Trans. on Computers, Vol. C-28, No. 9, pp. 660-670, Sept. 1979.	U. Banerjee, S. C. Chen, D. J. Kuck and R. A. Towle
	210	"The Use of Vocabulary Files for On-line Information Retrieval," Information Processing and Management, Vol. 15, No. 6, pp. 281-289, 1979.	T. G. Burket, P. Emrath and D. J. Kuck
1980	225	"High-Speed Multiprocessors and Compilation Techniques," Special Issue on Parallel Processing, IEEE Trans. on Computers, Vol. C-29, No. 9, pp. 763-776, Sept. 1980.	D. A. Padua, D. J. Kuck and D. H. Lawrie
1981	197	"On the Performance Enhancement of Paging Systems Through Program Analysis and Transformations," IEEE Trans. on Computers, Vol. C-30, No. 5, pp. 341-356, May 1981.	W. Abu-Sufah, D. J. Kuck, & D. H. Lawrie
	271	"A Bit-Serial/Tuple-Parallel Relational Query Processor," IBM Research Lab. Res. Rpt. No. RJ3194, San Jose, CA, July 1981.	Won Kim, David J. Kuck, & Daniel Gajski
1982	295	"A Second Opinion on Dataflow Machines and Languages," Invited paper, Special Dataflow Issue, IEEE Computer, Vol. 15, No. 2, pp. 58-69, Feb. 1982.	D. D. Gajski, D. A. Padua, D. J. Kuck, & R. H. Kuhn
	189	"The Burroughs Scientific Processor (BSP)," Special Issue on Supersystems, IEEE Trans. on Computers, Vol. C-31, No. 5, pp. 363-376, May 1982.	D. J. Kuck & Richard Stokes
1983	269	"Accessing Sparse Arrays in Parallel Memories," Journ. of VLSI and Computer Systems, Vol. 1, No. 1, pp. 69-100, Spring, 1983. (MCS76-81686, MCS80-01561, and US DOE DE-AC02-81ER10822)	U. Banerjee, D. Gajski, & D. Kuck

Name: Robert B. Wilhelmson

Date of Birth: September 15, 1944

Degrees	Institution	Date Conferred
B.S.	Wheaton College, Illinois	1966
M.S.	University of Illinois	1969
Ph.D.	University of Illinois	1972

Professional Experience:

Research Assistant, Computer Science Department, U. of Illinois, 1966-1969
Research Assistant, Laboratory for Atmospheric Research, 1969-1972
Research Assistant Professor, Laboratory for Atmospheric Research & Center for Advanced Computation, U. of Illinois, 1972-1974
Assistant Professor, Laboratory for Atmospheric Research & Center for Advanced Computation, U. of Illinois, 1974-1978
Associate Professor, Laboratory for Atmospheric Research, U. of Illinois, 1978-1983
Professor, Department of Atmospheric Sciences, U. of Illinois, 1983 to present

Professional Activities:

American Meteorological Society
American Scientific Affiliation
Member of the Storm Scale Working Group for SESAME 1979
Member of the Mesoscale Group during the Cyclone Project Workshop held in Seattle, 1979
Steering Committee for the Cumulus Dynamics and Microphysics Program initiated by NOAA, 1980-1982
Served on the SPEC review panel for the Scientific Computing Division of NCAR, 1981
Lectures and Notes on the Numerical Simulation of Convective Clouds given at the Symposium sponsored by the Cooperative Institute for Mesoscale Studies at the University of Oklahoma, May 12-16, 1980
Invited Reviews on the Simulation of Convection -
1980 - Fall American Geophysical Union Meeting
1981 - Fall American Geophysical Union Meeting
1982 - 12th Severe Storms Conference

Awards:

NCAR Outstanding Publication Award with Dr. Klemp, 1979
Meisinger Award from the American Meteorological Society with Dr. Klemp, 1983

Current Grants:

NOAA/NSSL Research Grant $10,000/yr., COMM NA82RAA00124
NSF Research Grant $273,434/2 yrs., Ogura/Wilhelmson, ATM-8210130

List of Publications — Robert Wilhelmson

Journals and books:

Wilhelmson, R., and Y. Ogura, 1972: The pressure perturbation and numerical modeling of clouds. J. Atmos. Sci., 29, 1295-1307.

Wilhelmson, R., 1974: The life cycle of a thunderstorm in three dimensions. J. Atmos. Sci., 31, 1629-1651.

Ericksen, J., and R. Wilhelmson, 1976: Implementation of a convection problem requiring auxiliary storage. ACM Trans. on Math. Software, 2, 187--195.

Wilhelmson, R., 1977: On the thermodynamic equation for deep convection. Mon. Wea. Rev., 105, 545-547.

Wilhelmson, R., and J. Ericksen, 1977: Direct solutions for Poisson's equation in three dimensions. J. Comput. Phys., 25, 319-331.

Klemp, J. B., and R. Wilhelmson, 1978: The simulation of three-dimensional convective storm dynamics. J. Atmos. Sci., 35, 1070-1096.

Wilhelmson, R., and J. B. Klemp, 1978: A numerical study of storm splitting that leads to long-lived storms. J. Atmos. Sci., 35, 1975-1986.

Klemp, J. B., and R. Wilhelmson, 1978: Simulations of right and left moving storms through storm splitting. J. Atmos. Sci., 35, 1097-1100.

Hane, C., R. Wilhelmson and T. Gal-Chen, 1981: Retrieval of thermodynamic variables within deep convective clouds: Experiments in three dimensions. Mon. Wea. Rev., 109, 564-576.

Klemp, J. B., R. B. Wilhelmson and P. S. Ray, 1981: Observed and numerically simulated structure of a mature supercell thunderstorm. J. Atmos. Sci., 38, 1558-1580.

Wilhelmson, R. B., and J. B. Klemp, 1981: A three-dimensional simulation of splitting severe storms on 3 April 1964. J. Atmos. Sci., 38, 1581--1600.

Ray, P. S., B. C. Johnson, K. W. Johnson, J. S. Bradberry, J. J. Stephens, K. K. Wagner, R. B. Wilhelmson and J. B. Klemp, 1981: The morphology of several tornadic storms on 20 May 1977. J. Atmos. Sci., 38, 1643-1663.

Wilhelmson, R. B., and C.-S. Chen, 1982: A simulation of the development of successive cells along a cold outflow boundary. J. Atmos. Sci., 39, 1466-1483.

Ray, P. S., R. B. Wilhelmson and K. W. Johnson, 1982: Model of a tornadic thunderstorm. Bull. Amer. Met. Soc., 63, 304.

Ray, P. S., J. B. Klemp and R. B. Wilhelmson, 1982: Observed and numerically simulated structure of a mature supercell thunderstorm. In Cloud Dynamics, ed. E. M. Agee and T. Asai, D. Reidel Publishing Company, pp. 379-393.

List of Publications Robert Wilhelmson

Other articles:

Wilhelmson, R. B., Abel et al., 1969: Tranquil: A language for array processing computer. Spring Joint Computer Conf., 57-B.

Wilhelmson, R. B., 1973: The life cycle of a thunderstorm--three dimensions. 8th Conf. on Severe Local Storms, 279-286.

Wilhelmson, R. B., 1974: Solving Partial Differential Equations using ILLIAC IV. Lecture Notes in Mathematics. Constructive and Computational Methods for Differential and Integral Equations. Symposium sponsored by the Air Force Office of Scientific Research, Indiana University, February 17-20, 453-476.

Klemp, J. B., and R. B. Wilhelmson, 1977: The simulation of three-dimensional convective storm dynamics. 10th Conf. on Severe Local Storms, 283-289.

Wilhelmson, R. B., and J. B. Klemp, 1978: The influence of microphysical processes on storm splitting and structure. Conf. on Cloud Physics and Atmospheric Electricity, 540-543.

Klemp, J. B., R. B. Wilhelmson, P. S. Ray, J. Stokes, B. Johnson, and K. Johnson, 1979: Comparison of modeled and observed severe storms. 11th Conf. on Severe Local Storms, 515-522.

Wilhelmson, R. B., and J. B. Klemp, 1979: The effect of gust fronts on the generation of multiple splitting storms. 11th Conf. on Severe Local Storms, 291-298.

Klemp, J. B., P. S. Ray, and R. B. Wilhelmson, 1980: Analysis of merging storms on 20 May 1977. 19th Conf. on Radar Meteor., 317-324.

Wilhelmson, R. B., 1980: Persistent storms obtained using a three-dimensional numerical storm model. Mini-symposium on Mesoscale Phenomena and Their Interactions held at the Geophysical Fluid Dynamics Laboratory, Princeton, New Jersey, 29.

Wilhelmson, R. B., 1980: Numerical Simulation of Convective Clouds. Collection of Lecture Notes on Dynamics of Mesometeorological Disturbances. CIMMS Symposium, University of Oklahoma, May 12-16, 261-379.

Droegemeier, K. K., and R. B. Wilhelmson, 1982: The roles of thunderstorm outflows in the production and maintenance of convection. 12th Conf. on Severe Local Storms, 516-519.

Wilhelmson, R. B., and C. S. Chen, 1982: Cell development along cold outflow boundaries. 12th Conf. on Severe Local Storms, 127-130.

Droegemeier, K. K., and R. B. Wilhelmson, 1983: Three-dimensional numerical simulation of interaction between a shallow cumulus field and a thunderstorm outflow boundary. 13th Conf. on Severe Local Storms.

Rasmussen, E. N., and R. B. Wilhelmson, 1983: Relationships between storm characteristics and 1200 GMT hodographs, low-level shear, and stability. 13th Conf. on Severe Local Storms.

Ray, P. S., J. B. Klemp, R. B. Wilhelmson, and K. W. Johnson, 1983: Testing of multiple-doppler analysis procedures from the synthesis of simulated radar scans. 21st. Conf. on Radar Meteorology.

Wilhelmson, R. B., and J. B. Klemp, 1983: Comparison of doppler and numerical model data of an Oklahoma squall line. 21st Conf. on Radar Meteorology.

Wilhelmson, R. B., and J. B. Klemp, 1983: Numerical simulation of severe storms within lines. 13th Conf. on Severe Local Storms.

Curriculum Vitae

July, 1983

PETER GUY WOLYNES

Department of Chemistry
University of Illinois
at Urbana-Champaign
Urbana, Illinois 61801

311 W. Oregon
Urbana, Illinois 61801
Phone: (217)328-6482

Born April 21, 1953 in Chicago, Illinois

Education:

Indiana University, A.B. (with highest distinction) with honors in Chemistry, 1971.

Phi Beta Kappa, Sigma Pi Sigma (physics honorary), Phi Lambda Upsilon (chemistry honorary), Sigma Xi.

Sigma Xi Undergraduate Research Award.

Harvard University, A.M. in chemistry, 1972, Ph.D. in chemical physics, March 1976. N.S.F. Fellow, 1971-74.

Professional Experience:

Indiana University Northwest, Teaching Assistant, Summer 1971

Harvard University, Teaching Fellow, Fall 1972, Spring 1973, 1974.

Massachusetts Institute of Technology, Research Associate, 1975-76.

Harvard University, Assistant Professor, 1976-1979
Associate Professor, 1979-1980

Max-Planck Institut für biophysikalische Chemie (Göttingen, FRG),
Visiting Scientist, Summer 1977.

University of Illinois, Associate Professor, 1980-1983

Alfred P. Sloan Fellow, 1981-1983

Institute for Molecular Science, Okazaki, Japan, Visiting Professor,
May-August, 1982

University of Illinois, Professor of Chemistry, 1983-present

Professional Activities:

Publications: see List.

Research Grants: ACS-PRF No. 9721-G6 (September 1977-September 1980/$9,000); NSF CHE 76-84224 (September 1977-February 1980/$57,100); NSF CHE 79-18568 (November 1979-February 1982/$70,000); NSF Instrumentation Grant NSF CHE-801903; Alfred P. Sloan Fellowship (1981-1983/$20,000); NSF CHE81-22012 (February 1982-February 1985/$221,417).

Society Membership. American Physical Society, American Association for the Advancement of Science, American Chemical Society.

Professional Activities (continued)

Graduate Instruction: Chem. 240 (H.U.) Statistical Mechanics, Chem. 442 (U.I.) Statistical Mechanics

Undergraduate Instruction: Nat Sci 3 (H.U.) Freshman Chemistry, Chem 160 (H.U.) Physical Chemistry.

Professional Meetings: Invited Lectures, see list.

Research Interests:

Chemical Physics, statistical mechanics.

Invited Lectures:

A. At Universities and Laboratories

Department of Chemistry, University of California, Berkeley-February, 1977.

Max-Planck Institut für biophysikalische Chemie-June, 1977.

Department of Chemistry, Purdue University-May, 1978.

Department of Chemistry, State University of New York at Stonybrook - October, 1978.

Department of Chemistry, Yale University - November, 1978.

Department of Chemistry, University of California, Los Angeles-January, 1979.

Department of Chemistry, Stanford University-January, 1979.

Department of Chemistry, University of California, Santa Barbara-January, 1979.

Department of Chemistry, Indiana University - February 1979.

Department of Chemistry, Columbia University-March, 1979.

Department of Chemistry, University of Illinois-April, 1979.

Department of Chemistry, Brandeis University (Rosenstiel Lecture)-May, 1979.

Department of Chemistry, University of Maine-October, 1979.

Department of Chemistry, Washington University-September, 1979.

Department of Chemistry, University of Houston-February, 1980.

Max-Planck-Institut für biophysikalische Chemie-October, 1979.

Thermal Physics Division, National Bureau of Standards-January, 1981.

Department of Chemistry, Colorado State University-March, 1981.

Department of Chemistry, University of Colorado-March, 1981.

Department of Physics, Technical University of Munich-September, 1981.

Invited Lectures (continued)

A. At Universities and Laboratories (continued)

Department of Chemistry, Rutgers University, New Brunswick, New Jersey - November, 1981

Department of Chemistry, Michigan State University, East Lansing, Michigan - March, 1982

Department of Chemistry, University of California, Berkeley - May, 1982

Department of Chemistry, Stanford University, Palo Alto, California - May, 1982

Institute for Molecular Science, Okazaki, Japan, June-July 1982

Department of Chemistry, Kyoto University, Kyoto, Japan July 1982

Department of Chemistry, Ochanomizou University, Tokyo, Japan, July 1982

Department of Chemistry, Keio University, Yokohama, Japan July 1982

Arrhenius Institute, University of Stockholm, Stockholm, Sweden, October, 1982

Department of Chemistry, Indiana University, Bloomington, Indiana, November 1982

Department of Chemistry, Columbia University, New York, November, 1982

B. At Professional Meetings

Special Session on Chemical Dynamics in Liquids, ACS Great Lakes Meeting, Indianapolis-May, 1978.

Gordon Conference on Dielectric Phenomena-August, 1978.

Symposium on Dynamics in Liquids, ACS-CSJ Meeting, Honolulu, Hawaii-April, 1979.

NRCC Workshop on Stochastic Molecular Dynamics, Woods Hole, Massachusetts-July, 1979.

Gordon Conference on Liquids-August, 1979

CECAM Workshop on Stochastic Dynamics with Hydrodynamic Interactions, Bilthoven, The Netherlands-October, 1979

NRCC Workshop on Simulations with Long Range Forces, Palo Alto, California-January, 1980.

Gordon Conference on Water--August, 1980

American Physical Society - Symposium on Chemical and Biological Reaction Rates-March, 1981

Invited Lectures (continued)

American Chemical Society - Symposium on Dynamics of Solutions-April, 1981

4th American Theoretical Chemistry Conference-June, 1981

Gordon Conference on Molecular Energy Transfer-June, 1981

Gordon Conference on Liquids, Holderness, New Hampshire - August, 1981

American Chemical Society - Symposium on New Ideas in Chemical Kinetics, New York - August, 1981

Hungarian Academy of Sciences - Conference on Quantum Dynamics of Complex Molecules, Szeged, Hungary - September, 1981

XI Reunion de Fisica Estadistica, Cocoyoc, Mexico - January, 1982

American Physical Society, Dallas, Texas - March, 1982

6th International Symposium on Solute-Solute-Solvent Interactions, Minoo, Osaka Japan, July 1982

American Chemical Society, Kansas City, September, 1982

Nobel Symposium on Biomolecular Dynamics, Gysinge, Sweden, October, 1982

NATO-CECAM Conference on Quantum Monte Carlo Methods, Paris- France - December, 1982

est Foundation Physics Conference, San Francisco, California - January, 1983

American Chemical Society, Symposium on Structure and Dynamics of Liquids, Seattle, Washington - March, 1983

International Center for Theoretical Physics, Conference on Quantum Monte Carlo Methods, Trieste, Italy - July 1983

Symposia Chaired:

Sessions at

Texas Conference on Theoretical Approaches to Chemical Dynamics - March, 1981

American Chemical Society - Symposium on Dynamics of Solutions - June, 1981

American Chemical Society, Symposium on Structure and Dynamics of Liquids, Seattle, Washington - March, 1983

COURSES TAUGHT:

Graduate Instruction:

Chem 441 (U.I.) Thermodynamics & Statistical Thermodynamics

443 (U.I.) Quantum Dynamics

Undergraduate Instruction:

Chem 344 (U.I.) Physical Chemistry II

Publications

1. Bounds for Convective Contributions to Transport Coefficients, P. G. Wolynes, Phys. Rev. A11, 1700 (1975).

2. Hydrodynamic Boundary Conditions and Mode-Mode Coupling Theory, P. G. Wolynes, Phys. Rev. A13, 1235 (1976).

3. Osmotic Effects near the Critical Point, P. G. Wolynes, J. Phys. Chem. 80, 1570 (1976).

4. Slip Boundary Conditions and the Hydrodynamic Effect on Diffusion-Controlled Reactions, P. G. Wolynes and J. M. Deutch, J. Chem. Phys. 65, 450 (1976).

5. Hydrodynamic Boundary Conditions and Polymer Dynamics, P. G. Wolynes and J. M. Deutch, J. Chem. Phys. 65, 2030 (1976).

6. The Hinge-Bending Mode of Lysozyme, J. A. McCammon, B. R. Gelin, M. Karplus and P. G. Wolynes, Nature 262, 325 (1976).

7. Hydrodynamic Effect on the Coagulation of Porous Biopolymers, P. G. Wolynes and J. A. McCammon, Macromolecules, 10, 86 (1977).

8. Nonsteady Hydrodynamics of Biopolymer Motions, J. A. McCammon and P. G. Wolynes, J. Chem. Phys. 66, 1452 (1977).

9. Dynamical Orientation Correlations in Solution, P. G. Wolynes and J. M. Deutch, J. Chem. Phys., 67, 733 (1977).

10. On the Effects of Translation-Rotation Coupling on Hydrodynamic Diffusion Tensors, J. A. Montgomery, Jr., B. J. Berne, P. G. Wolynes, and J. M. Deutch, J. Chem. Phys. 67, 5971 (1977).

11. Molecular Theory of Solvated Ion Dynamics, P. G. Wolynes, J. Chem. Phys. 68, 473 (1978).

12. Molecular Interpretation of the Infrared Water Vapor Continuum, P. G. Wolynes and R. E. Roberts, Applied Optics, 17, 1484 (1978).

13. Semiclassical Description of Electron Spin Motion in Radicals Including the Effect of Electron Hopping, K. Schulten and P. G. Wolynes, J. Chem. Phys. 68, 3292 (1978).

14. Dielectric Friction and Molecular Reorientation, J. B. Hubbard and P. G. Wolynes, J. Chem. Phys. 69, 998 (1978).

15. Relaxation Processes and Chemical Kinetics, J. L. Skinner and P. G. Wolynes, J. Chem. Phys, 69, 2143 (1978).

16. Picosecond Dynamics of Tyrosine Sidechains in Proteins, J. A. McCammon, P. G. Wolynes and M. Karplus, Biochemistry, 18, 927 (1979).

17. Ionic Mobility: Theory Meets Experiment, T. Tomimaga and D. F. Evans, J. B. Hubbard, P. G. Wolynes, J. Phys. Chem. 83, 2669 (1979).

18. Derivation of Smoluchowski Equations with Corrections for Fokker-Planck and BGK Collision Models, J. L. Skinner and P. G. Wolynes, Physica, 96A, 561 (1979).

19. Molecular Theory of Solvated Ion Dynamics II: Local Structure and Ionic Mobility, P. Colonomos and P. G. Wolynes, J. Chem. Phys, 71, 2644 (1979).

20. Molecular Theory of Solvated Ion Dynamics III: Dielectric Decrement, J. B. Hubbard, P. Colonomos and P. G. Wolynes, J. Chem. Phys. 71, 2652 (1979).

21. What's Simple about Complex Fluids?, P. G. Wolynes (translated by T. Fujiyama), Kagaku no Ryoiki (Journal of Japanese Chemistry), 33, 897 (1979).

22. Flow Birefringence and Hydrodynamic Boundary Conditions, D. F. Calef and P. G. Wolynes, J. Chem. Phys., 72, 535 (1980).

23. General Kinetic Models of Activated Processes in Condensed Phases, J. L. Skinner and P. G. Wolynes, J. Chem. Phys. 72, 4913 (1980).

24. Dynamics of Electrolyte Solutions, P. G. Wolynes, Ann. Rev. Phys. Chem. 31, 345 (1980).

25. Transition State and Brownian Motion Theories of Solitons, J. L. Skinner and P. G. Wolynes, J. Chem. Phys. 73, 4015 (1980).

26. Solitons, Defect Diffusion, and Dielectric Relaxation of Polymers, J. L. Skinner and P. G. Wolynes, J. Chem. Phys. 73, 4022 (1980).

27. Impulsive Stochastic Models of Molecular Relaxation and Isomerization Reactions, B. J. Berne, J. L. Skinner and P. G. Wolynes, J. Chem. Phys. 73 4314 (1980).

28. Exploiting the Isomorphism Between Quantum Theory and the Classical Statistical Mechanics of Polyatomic Fluids, D. Chandler and P. G. Wolynes, J. Chem. Phys. 74, 4078 (1981).

29. A Continuum Theory for Quadrupole Relaxation of Ions in Solution, J. T. Hynes and P. G. Wolynes, J. Chem. Phys. 75, 395 (1981).

30. Convenient and Accurate Discretized Path Integral Methods for Equilibrium Quantum Mechanical Calculations, K. Schweizer, R. Stratt, D. Chandler and P. G. Wolynes, J. Chem. Phys. 75, 1347 (1981).

31. Quantum Theory of Activated Events in Condensed Phases, P. G. Wolynes, Phys. Rev. Lett., 47, 968 (1981).

32. An Electrohydrodynamic Contribution to the Hall Effect in Electrolyte Solutions, J. B. Hubbard and P. G. Wolynes, J. Chem. Phys. 75, 3051 (1981).

33. NMR Relaxation Parameters in Molecules with Internal Motion: Exact Langevin Trajectory Results Compared with Simplified Relaxation Models, R. M. Levy, M. Karplus and P. G. Wolynes, J. Am. Chem. Soc. 103, 599 (1981).

34. Smoluchowski-Vlasov Theory of Charge Solvation Dynamics, D. Calef and P. G. Wolynes, J. Chem. Phys. 78, 4145 (1983).

35. Book Review: Functional Integration: Theory and Applications, P. G. Wolynes, J. Stat. Phys. 28, 409 (1982).

36. Quantum Statistical Mechanics of Solvation, P. G. Wolynes, in Proceedings of 6th International Symposium on Solute-Solute-Solvent Interactions, H. Ohtakhi, editor, Elsevier Press, to appear.

37. Classical Solvent Dynamics and Electron Transfer I. Continuum Theory, D. F. Calef and P. G. Wolynes, J. Phys. Chem., to appear.

38. Classical Solvent Dynamics and Electron Transfer II. Molecular Theory, D. F. Calef and P. G. Wolynes, J. Chem. Phys., 78, 470 (1983).

39. Surface Roughness, Hydrodynamic Boundary Conditions and Electrophoresis, R. W. Wunderlich and P. G. Wolynes, J. Fluid Mech., submitted for publication.

40. Electronic States of a Topologically Disordered System: Exact Solution of the Mean Spherical Model for Liquids, D. Chandler, K. S. Schweizer, and P. G. Wolynes, Phys. Rev. Lett. 49, 1100 (1982).

41. Renormalization Group Studies of Tunneling Systems, G. A. Jongeward and P. G. Wolynes, J. Chem. Phys., to appear.

42. Chemical Physics of Molecular Systems in Condensed Phases, P. G. Wolynes in Proceedings of NATO Workshop on Monte Carlo Methods for Quantum Problems, M. Kalos ed., (Dordrecht, to appear 1984).

VITA

Karl Hess was born in Trumau, Austria, on June 20, 1945. After studying physics and mathematics he received his Ph.D. degree (Dr. Phil.) at the University of Vienna, Austria in 1970.

In 1969 he became associated with the University of Vienna and the Boltzmann Institute as a Research Assistant. In 1971 he was promoted to Assistant Professor and in 1977 Universitätsdozent. He was a Visiting Assistant Professor at the University of Illinois at Urbana-Champaign during the academic year 1973/74 and returned to the University of Illinois in 1977, where he is currently Professor of Electrical Engineering and Research Professor in the Coordinated Science Laboratory. In 1982 he was named a Beckmann Associate in the Center for Advanced Study.

Dr. Hess has done research on the Hf conductivity of semiconductors, the acoustoelectric effect, hot electrons and MOS devices, and transport problems in CCD's. He is presently interested in electronic properties of quantum well heterostructures and superlattices.

Dr. Hess is a senior member of IEEE and the American Physical Society. He has served as a committee member of many national and international conferences and presently serves on a recommendation committee for the National Research Council.

PERSONAL DATA

Born:	June 20, 1945 in Trumau, Lower Austria Son of Karl and Gertrude Hess
Education:	Elementary school and high school in Baden, Austria
	Abitur on July 4, 1963 (general certificate of education at the advanced level)
	Studies of physics and mathematics at the University of Vienna, Ph.D. thesis on energy relaxation in semiconductors (1967-1970), Ph.D. on November 10, 1970.
Marriage:	Sylvia Horvath on September 31, 1967
Children:	Ursula, April 24, 1968 Karl, January 13, 1971

MAJOR RESEARCH PROJECTS

1. Microwave Techniques in Semiconductor Physics - Hot Electrons (1970-1972)
2. Acoustoelectric Effect (1971-1973)
3. Infrared Optics (1974-1976)
4. MOS-Transistor - Hot Electrons (1973-1977)
5. High Magnetic Fields - Semiconductors (1975-1977)
6. Transport Properties of p-Silicon and p-Germanium Under Uniaxial Pressure (1975-1977)
7. Nonstationary Noise in Charge-Coupled Devices (1977-1978)
8. Ion Implantation and Deep Levels of Structural Defects (1978-1979)
9. Transport Properties of Quantum Well Heterostructures (1979-present)
10. Impact Ionization Phenomena in Semiconductors (present)
11. Physics of Submicron Devices (1979-present)

INVITED LECTURES

1. "Hot Carriers in MOSFET's in High Magnetic Fields",
   International Conference on the Application of High Magnetic Fields in Semiconductor Physics,
   Würzburg, Germany, August 1976.

2. "Review of Experimental Aspects of Hot Electron Transport in MOS Structures",
   International Conference on Hot Electrons in Semiconductors,
   Denton, Texas, July 1977.

3. "Hot Electron Transport in Surface Inversion Layers",
   International Conference on Two Dimensional Systems,
   Berchtesgaden, Germany, September 1977.

4. "Hot Electron Phenomena in MOS Structures",
   Workshop on Hot Electron Phenomena in Semiconductors,
   Cornell University, Ithaca, New York, August 1978.

5. "Physics of Nonlinear Transport in Semiconductors",
   NATO Advanced Study Institute,
   Sogesta, Urbino, Italy, July 1979.

6. "Real Space Transfer of Hot Electrons in Modulation-Doped Structures",
   March Meeting of the American Physical Society,
   New York, 1980.

7. "Scattering Mechanisms at Interfaces",
   Workshop on the Physics of Submicron Structures,
   Fort Collins, Colorado, 1980.

8. "High Field, Transport in Fineline Semiconductor Devices",
   Device Research Conference,
   Santa Barbara, California, 1981.

9. "Lateral Transport in Superlattices",
   3rd International Conference on Hot Electrons in Semiconductors,
   Montpellier, France, 1981.

10. "Electronic Transport in Heterojunctions and Superlattices",
    16th International Conference on the Physics of Semiconductors,
    Montpellier, France, September 6-10, 1982.

11. "Electronic Transport in GaAs-GaAlAs Heterolayers and High Mobility Transistors",
    General Meeting of the American Physical Society,
    Philadelphia, November 3-5, 1982.

12. "The Boltzmann Transport Equation", and
"Superlattices",
NATO Advanced Study Institute,
San Miniato, Italy, Summer 1983.

13. "Emission and Capture of Electrons in Quantum Wells:
Lasers and Modulation-doped Heterolayer Structures",
Rank Prize Fund Symposium on Optical and Opto-electronic Properties
of Semiconductor Multi-Layer Structures,
Malvern, England, Summer 1983.

M.S. AND Ph.D. GRADUATES

Hisashi Shichijo (1980) Ph.D.: "Theoretical Studies of High Field Transport in III-V Semiconductors."
Current Employer: Texas Instruments

Henry Kafka (1980) M.S.: "An Electron Temperature Model for IMPATT Diodes."
Current Employer: Bell Laboratories

J. Y. Tang (1980), M.S.: "Real Space Transfer Noise in Semiconductor Devices."

M. S. Burroughs (1981) M.S.: "Effects of Alloy Clustering in III-V Semiconductor Compounds."
Current Employer: GTE

W. T. Jones (1981) M.S.: "Electronic Diffusion in Semiconductor Devices."
Current Employer: Bell Laboratories

J. Y. Tang (1982) Ph.D.: "Theoretical Studies of High Field, High Energy Transport in GaAs, Si and Heterostructures."
Current Employer: IBM

Mark R. Keever (1982) Ph.D.: "Experimental Studies of Lateral Electron Transport in Gallium Arsenide-Aluminum Gallium Arsenide Heterostructures."
Current Employer: Hewlett-Packard

PROFESSIONAL ACTIVITIES AND HONORS

Conference Organizations

Solid State Devices Committee of the IEDM, 1981.
Solid State Devices Committee of the IEDM, 1982.
Chairman, Workshop on the Physics of Submicron Structures, University of Illinois, Allerton House, Urbana, Illinois, June 1982.
Fourth International Conference on Electronic Properties of Two-Dimensional Systems, New Hampshire, August 1981.
Third International Conference on Hot Carriers in Semiconductors, Montpellier, France, July 1981.
International Conference on Metastable and Modulated Semiconductor Structures, Pasadena, December 1982.

National Committees

Electronics Committee on Recommendations for U. S. Army Basic Scientific Research, National Research Coundil

Consultant

U. S. Army, Ft. Monmouth
Naval Research Laboratory
Previous consultant for various electronics companies: Siemens (Germany), Gould (Chicago), and others

Honors

Fulbright Scholar 1973/74
Beckmann Associate 1982/83
Center for Advanced Study, University of Illinois, Urbana, IL
Included in: Who's Who in Technology Today
Who's Who in the Midwest

Patent

United States Patent No. 4,257,055:
Negative Resistance Heterojunction Devices,
Karl Hess et al., March 17, 1981.

1. K. Hess and K. Seeger, "Energie-Relaxation warmer Ladungstrager in Germanium und Silizium," Z. Physik 218, 431-436 (1968).

2. K. Hess, G. Nimtz, and K. Seeger, "Non-Ohmic Microwave Conductivity in Semiconductor Posts," Solid-State Electronics 12, 79-84 (1969).

3. H. Kahlert, K. Hess and K. Seeger, "Energy Relaxation of Warm Holes in p-Type Tellurium," Solid State Communications 7, 1149-1152 (1969).

4. K. Seeger and K. Hess, "Momentum and Energy Relaxation of Warm Carriers in Semiconductors," Z. Physik 237, 252-262 (1970).

5. K. Hess and H. Kahlert, "Harmonic Mixing and Energy Relaxation of Warm Electrons in n-GaAs at Low Temperatures," J. Phys. Chem. Solids 32, 2262-2265 (1970).

6. H. Kuzmany and K. Hess, "Mode Development in the Cadmium Sulphide Acousto-Electric Oscillator," Phys. Stat. Sol. (a) 4, 417-425 (1971).

7. H. Kuzmany and K. Hess, "Influence of the Second Harmonic on the Acousto-Electric Gain in Piezoelectric Semiconductors," Phys. Stat. Sol. (a) 7, K21-K23 (1971).

8. K. Hess, "Effect of Uniaxial Stress on Energy Loss and Scattering Mechanism in p-Type Silicon," J. Phys. Chem. Solids 33, 139-143 (1972).

9. H. Heinrich, K. Hess, W. Jantsch and W. Pfeiler, "Determination of the Energy Relaxation Time in GaSb from Microwave Harmonic Mixing and Transport Phenomena," J. Phys. Chem. Solids, 33, 425-431 (1972).

10. K. Hess and H. Kuzmany, "Determination of Absolute Values for the Piezoelectric Potential and Carrier Distribution in Acoustic Domains by a Combination of Microwave Absorption and Brillouin Scattering," Proc. Int. Conf. Physics of Semicond., 1233-1237, Warsaw, July 25-29 (1972).

11. K. Hess and H. Kuzmany, "Nonlinear Solution for Single-Mode Operated Acousto-Electric Oscillators," Phys. Stat. Sol. (a) 9, 253-258 (1972).

12. K. Hess and H. Kuzmany, "Microwave Absorption by Bunched Carriers in Acoustoelectric Domains," J. Phys. C: Solid State Phys. 6, 657-670 (1973).

13. K. Hess and H. Vana, "Deviations from Ohm's Law in n-CdS at 77 K," J. Phys. C: Solid State Phys. 6, L150-L151 (1973).

14. K. Hess and H. Kuzmany, "Infrared Absorption by Acoustoelecric Domains in ZnO," J. Phys. C: Solid State Phys. 6, L376-L378 (1973).

15. K. Hess and C. T. Sah, "Hot Carriers in Silicon Surface Inversion Layers," J. Appl. Phys. 45 (3), 1254-1257 (1974).

16. J. Dow, M. Bowen, R. Bray, D. L. Spears, and K. Hess, "Piezo-Urbach Rule for Acoustoelectric Domains in GaAs," Physical Review B 10 (10), 4305-4308 (1974).

17. K. Hess and C. T. Sah, "High Frequency Hot Electron Conductivity and Admittance in Si and Ge," Solid State Electronics 18, 667-669 (1974).

18. K. Hess and C. T. Sah, "Warm and Hot Carriers in Silicon Surface-Inversion Layers," Physical Review B 10 (8), 3375-3386 (1974).

19. K. Hess, A. Neugroschel, C. C. Shiue, and C. T. Sah, "Non-Ohmic Electron Conduction in Silicon Surface Inversion Layers at Low Temperatures," J. Appl. Phys. 46 (4), 1721-1727 (1975).

20. K. Hess and C. T. Sah, "Dipole Scattering at the Si-SiO_2 Interface," Surf. Sci. 47, 650-654 (1975).

21. K. Hess, "Hot-Electron Magnetoresistance in n-Silicon Inversion Layers," Phys. Stat. Sol. (a) 31, 483-487 (1975).

22. K. Hess, "On the Magnetoresistance of Silicon Surface Inversion Layers," Phys. Stat. Sol. (a) 31, 159-164 (1975).

23. K. Hess, "Anisotropic Impurity Scattering in Electrically Quantized Inversion Layers," Solid State Comm. 17, 157-159 (1975).

24. K. Hess, "Magnetcresistance of n-Silicon Inversion Layers in the Ohmic and in the Hot-Electron Range," Surf. Sci. 58, 235-237 (1976).

25. F. Kuchar, E. Fantner, and K. Hess, "Ionized Impurity Scattering in Semiconductors: InSb Doped by Neutron Irradiation," J. Phys. C: Solid State Phys. 9, 3165-3171 (1976).

26. K. Hess, G. Dorda, and C. T. Sah, "The Current-Voltage Characteristics of Field-Effect Transistors with Short Channels," Solid State Comm. 19, 471-473 (1976).

27. E. Vass and K. Hess, "Energy Loss of Warm and Hot Carriers in Surface Inversion Layers of Polar Semiconductors," Z. Physik B25, 323-325 (1976).

28. K. Hess, T. Englert, T. Neugebauer, G. Landwehr, and G. Dorda, "Non-Ohmic Effects in p-Type Silicon Inversion Layers," Proc. XIII Int. Conf. on the Physics of Semiconductors, Rome, August 1976.

29. K. Hess, "Hot Carriers in MOSFETs in High Magnetic Fields," Int. Conf. on "The Application of High Magnetic Fields in Semiconductor Physics," Wurzburg, August 1976.

30. M. Sweid and K. Hess, "Frequency Dependent Microwave Absorption in Acoustoelectric Domains in ZnO," Z. Physik B24, 327-332 (1977).

31. K. Hess, "Transporteigenschaften von Feldeffekt-Transistoren," Acta Physica Austriaca 47, 31-57 (1977).

32. G. Dorda, I. Eisele, E. Soutschek, E. Vass, and K. Hess, "Electron Transport at the Si-SiO_2 Interface," Proc. 7th Intern. Vac. Congr. and 3rd Intern. Conf. Solid Surfaces, pp. 563-565 (1977).

33. K. Hess, T. Englert, T. Neugebauer, G. Landwehr, and G. Dorda, "Hot-Carrier Effects in High Magnetic Fields in Silicon Inversion Layers at Low Temperatures: p Channel," Phys. Rev. B 16 (8), 3652-3659 (1977).

34. M. Sweid, K. Hess and K. Seeger, "Energy and Momentum Relaxation of Charge Carriers in Ge and Si under Uniaxial Stress," J. Phys. Chem. Solids 39, 393-402 (1978).

35. T. Neugebauer, G. Landwehr, and K. Hess, "Negative Differential Resistance in (100) n-Channel Silicon Inversion Layers," Solid-State Electronics 21 (1), 143-146 (1978).

36. K. Hess, "Review of Experimental Aspects of Hot Electron Transport in MOS Structures," Solid State Electronics 21, 123-132 (1978).

37. K. Hess, "Energy Relaxation to Acoustic Phonons in Surface Inversion Layers," Solid State Comm. 25, 191-192 (1978).

38. K. Hess and C. T. Sah, "Hot Electrons in Short-Gate Charge-Coupled Devices," IEEE Trans. on Electron Devices ED-25 (12), 1399-1405 (1978).

39. D. S. Day, M. J. Helix, K. Hess, and B. G. Streetman, "Deep Level Transient Spectroscopy for Diodes with Large Leakage Currents," Rev. Sci. Instrum. 50 (12), 1571-1573 (1979).

40. K. Hess, "Impurity and Phonon Scattering in Layered Structures," Appl. Phys. Lett. 35 (7), 484-486 (1979).

41. K. Hess and P. Vogl, "Remote Polar Phonon Scattering in Silicon Inversion Layers," Solid State Comm. 30, 807-809 (1979).

42. K. Hess, J. F. Detry, and C. T. Sah, "Trapping Noise in Charge Coupled Devices," Phys. Stat. Sol. (a) 55, 243-249 (1979).

43. K. Hess and C. T. Sah, "The Ultimate Limits of CCD Performance Imposed by Hot Electron Effects," Solid State Electronics 22, 1025-1033 (1979).

44. K. Hess, H. Morkoç, H. Shichijo, and B. G. Streetman, "Negative Differential Resistance Through Real-Space Electron Transfer," Appl. Phys. Lett. 35 (6), 469-471 (1979).

45. R. M. Kolbas, N. Holonyak, Jr., B. A. Vojak, K. Hess, M. Altarelli, R. D. Dupuis, and P. D. Dapkus, "Phonon Assisted Recombination and Stimulated Emission in Multiple Quantum-Well MO-CVD $Al_xGa_{1-x}As$-GaAs Heterostructures," Solid State Comm. 31, 1033-1037 (1979).

46. K. Hess, "Impurity and Phonon Scattering in Layered Structures," Appl. Phys. Lett. 35 (7), 484-486 (Oct. 1979).

47. K. Hess, "Phenomenological Physics of Hot Carriers in Semiconductors," Physics of Nonlinear Transport in Semiconductors, eds. D. K. Ferry, J. R. Barker and C. Jacoboni, pp. 1-42 (1980).

48. K. Hess, N. Holonyak, Jr., W. D. Laidig, B. A. Vojak, J. J. Coleman, and P. D. Dapkus, "Hot Electrons and Phonons in Quantum-Well $Al_xGa_{1-x}As$-GaAs Heterostructures," Solid State Communications 34, 749-752 (1980).

49. K. Hess and H. Shichijo, "The Charge-Handling Capacity of Buried-Channel Structures under Hot-Electron Conditions," IEEE Trans. on Electron Devices ED-27 (2), 503-504 (1980).

50. J. J. Coleman, P. D. Dapkus, B. A. Vojak, W. D. Laidig, N. Holonyak, Jr., and K. Hess, "Induced Phonon-Sideband Laser Operation of Large Quantum Well $Al_xGa_{1-x}As$-GaAs Heterostructures," Appl. Phys. Lett. 37 (1), 15-17 (1980).

51. K. Hess, B. A. Vojak, N. Holonyak, Jr., R. Chin, and P. D. Dapkus, "Temperature Dependence of Threshold Current for a Quantum-Well Heterostructure Laser," Solid State Electronics 23, 585-589 (1980).

52. N. Holonyak, Jr., R. M. Kolbas, W. D. Laidig, B. A. Vojak, K. Hess, R. D. Dupuis, and P. D. Dapkus, "Phonon-Assisted Recombination and Stimulated Emission in Quantum Well $Al_xGa_{1-x}As$-GaAs Heterostructures, Appl. Phys. Lett. 51 (3), 1328-1337 (1980).

53. H. Shichijo, K. Hess and G. E. Stillman, "Orientation Dependence of Ballistic Electron Transport and Impact Ionization," Electronics Letters 16 (6), 208-210 (1980).

54. K. Hess, "Real Space Transfer of Hot Electrons in Modulation-Doped Structures," Meeting of the American Physical Society, New York, March 1980.

55. N. Holonyak, Jr., B. A. Vojak, W. D. Laidig, K. Hess, J. J. Coleman, and P. D. Dapkus, "Phonon Contribution to Double-Heterojunction Laser Operation," Appl. Phys. Lett. 37 (2), 136-138 (1980).

56. B. A. Vojak, N. Holonyak, Jr., W. D. Laidig, K. Hess, J. J. Coleman, and P. D. Dapkus, "The Exciton in Recombination in $Al_xGa_{1-x}As$-GaAs Quantum-Well Heterostructures," Solid State Communications 35, 477-481 (1980).

57. R. Chin, N. Holonyak, Jr., B. A. Vojak, K. Hess, R. D. Dupuis, and P. D. Dapkus, "Temperature Dependence of Threshold Current for Quantum Well $Al_xGa_{1-x}As$-GaAs Heterostructure Laser Diodes," Appl. Phys. Lett. 36 (1), 19-21 (1980).

58. H. Shichijo, K. Hess, and B. G. Streetman, "Real-Space Electron Transfer by Thermionic Emission in GaAs-$Al_xGa_{1-x}As$ Heterostructures: Analytical Model for Large Layer Widths," Solid State Electronics 23, 817-822 (1980).

59. T. H. Glisson, J. R. Hauser, M. A. Littlejohn, K. Hess, B. G. Streetman, and H. Shichijo, "Monte Carlo Simulation of Real-Space Electron Transfer in GaAs-AlGaAs Heterostructures," J. Appl. Phys. 51 (10), 5445-5449 (1980).

60. R. Chin, N. Holonyak, Jr., G. E. Stillman, J. Y. Tang, and K. Hess, "Impact Ionization in Multilayered Heterojunction Structures," Electronics Letters 16 (12), 467-469 (1980).

61. K. K. Mon and K. Hess, "Electron-Phonon Interaction at Semiconductor Interfaces," Workshop on Artificial Superlattices, University of Illinois (Oct. 1980).

62. K. Hess and N. Holonyak, Jr., "Hot Electrons in Layered Semiconductor Structures," Physics Today, Oct. 1980, pp. 90-98.

63. N. Holonyak, Jr., W. D. Laidig, B. A. Vojak, K. Hess, J. J. Coleman, P. D. Dapkus, and J. Bardeen, "Alloy Clustering in $Al_xGa_{1-x}As$-GaAs Quantum-Well Heterostructures," Phys. Rev. Lett. 45, 1703 (1980).

64. H. Shichijo, K. Hess, and G. E. Stillman, "Simulation of High Field Transport in GaAs using a Monte Carlo Method and Pseudopotential Band Structures," Applied Physics Letters 38 (2), 89-91 (Jan. 1981).

65. M. Keever, H. Shichijo, K. Hess, S. Banerjee, L. Witkowski, H. Morkoç, and B. G. Streetman, "Measurements of Hot Electron Conduction and Real-Space Transfer in GaAs-$Al_xGa_{1-x}As$ Heterojunction Layers," Applied Physics Letters 38, 36-38 (Jan. 1981).

66. M. Keever, T. Drummond, K. Hess, H. Morkoç, and B. G. Streetman, "Time Dependence of the Current at High Electric Fields in $Al_xGa_{1-x}As$-GaAs Heterojunction Lasers," Electronics Letters 17 (2), 93-94 (Jan. 1981).

67. B. A. Vojak, N. Holonyak, Jr., W. D. Laidig, K. Hess, J. J. Coleman, and P. D. Dapkus, "Phonon Contribution to Metalorganic Chemical Vapor Deposited $Al_xGa_{1-x}As$-GaAs Quantum-Well Heterostructure Laser Operation," J. of Appl. Phys. 52 (2), 959-968 (Feb. 1981).

68. H. Shichijo and K. Hess, "Band Structure Dependent Transport and Impact Ionization in GaAs," Phys. Rev. B 23, 4197-4207 (April 1981).

69. A. Bhattacharyya, B. G. Streetman, and K. Hess, "Theoretical and Experimental Investigation of the Dynamics of Pulsed Laser Annealing," Journal of Applied Physics 52, 3611-3617 (May 1981).

70. J. Y. Tang and K. Hess, "Real Space Transfer Noise in Buried Channel Devices," IEEE Trans. on Electron Devices ED-28 (3), 285-289 (1981).

71. W. D. Laidig, N. Holonyak, Jr., M. D. Camras, K. Hess, J. J. Coleman, P. D. Dapkus, and J. Bardeen, "Disorder of an AlAs-GaAs Superlattice by Impurity Diffusion," Appl. Phys. Lett. 38 (10), 776-778 (May 1981).

72. T. J. Drummond, M. Keever, W. Kopp, H. Morkoç, K. Hess, B. G. Streetman, and A. Y. Cho, "Field Dependence of Mobility in $Al_{0.2}Ga_{0.8}As$/GaAs Heterojunctions at Very Low Fields," Electronics Letters 17 (15), 545-546 (July 1981).

73. J. Y. Tang, H. Shichijo, K. Hess, and G. Iafrate, "Band-Structure Dependent Impact Ionization in Silicon and Gallium Arsenide," Proc. 3rd Int. Conf. on Hot Electrons in Semiconductors, Montpellier, France (1981).

74. H. Kafka and K. Hess, "A Carrier Temperature Model Simulation of a Double-Drift IMPATT Diode," IEEE Trans. on Electron Devices, ED-28, 831 (1981).

75. P. D. Dapkus, J. J. Coleman, W. D. Laidig, N. Holonyak, Jr., B. A. Vojak, and K. Hess, "Continuous Room Temperature Laser Operation of Photopumped $Al_xGa_{1-x}As$-GaAs Superlattices," Applied Physics Letters 38, 118-120 (1981).

76. D. K. Ferry, K. Hess, and P. Vogl, "Physics and Modeling of Submicron Insulated-Gate Field-Effect Transistors. II. Transport in the Quantized Inversion Layer," Microstructure Science and Technology/VLSI, pp. 67-104, Norman Einspruch, Editor, (New York: Academic Press,1981).

77. W. D. Laidig, N. Holonyak, Jr., M. D. Camras, B. A. Vojak, K. Hess, J. J. Coleman, and P. D. Dapkus, "Quenching of Stimulated Phonon Emission in $Al_xGa_{1-x}As$-GaAs Quantum-Well Heterostructures," Solid State Commun. 38 (4), 301-304 (1981).

78. N. Holonyak, Jr., W. D. Laidig, K. Hess, J. J. Coleman, and P. D. Dapkus, "Comments: Alloy Clustering in $Al_xGa_{1-x}As$; Holonyak, et al., Respond," Phys. Rev. Lett. 46, 1042-1043 (1981).

79. K. Hess, "Ballistic Electron Transport in Semiconductors," IEEE Trans. on Electron Devices, ED-28, 937 (1981).

80. K. Hess and N. Holonyak, Jr., "Hot-Electron and Phonon Effects in Layered Semiconductor Structures and Heterostructures," Comments on Solid State Physics, 10, 67 (1981).

81. K. K. Mon, K. Hess, and John D. Dow, "Deformation Potentials of Superlattices and Interfaces," J. Vac. Sci. and Technology 19, 564-566 (1981).

82. T. J. Drummond, H. Morkoç, K. Hess, and A. Y. Cho, "Experimental and Theoretical Electron Mobility of Modulation Doped $Al_xGa_{1-x}As$/GaAs Heterostructures Grown by Molecular Beam Epitaxy," Journal of Applied Physics 52, 5231-5234 (1981).

83. T. J. Drummond, W. Kopp, H. Morkoç, K. Hess, A. Y. Cho, and B. G. Streetman, "Effect of background doping on the electron mobility of (Al,Ga)As/GaAs heterostructures," J. Appl. Phys. 52, 5689-5690 (1981).

84. M. Keever, T. J. Drummond, H. Morkoç, K. Hess and B. G. Streetman, "High Field Transport in GaAs-$Al_xGa_{1-x}As$ Heterojunction Layers," IEEE-Device Research Conf., Santa Barbara, 1981 and IEEE Trans. on Electron Dev. ED-28, 1233 (1981).

85. K. Hess and J. D. Dow, "Deformation Potentials of Bulk Semiconductors," Solid State Communications 40, 371 (1981).

86. N. Holonyak, Jr., W. D. Laidig, M. D. Camras, K. Hess, M. S. Burroughs, J. J. Coleman and P. D. Dapkus, "Size Fluctuations and High Energy Laser Operation of $Al_xGa_{1-x}As$-AlAs-GaAs Quantum Well Heterostructures," J. of Appl. Phys. 52, 6777 (1981).

87. N. Holonyak, Jr., W. D. Laidig, M. D. Camras, H. Morkoç, T. J. Drummond, K. Hess, and M. S. Burroughs, "Clustering in MBE $Al_xGa_{1-x}As$-GaAs Quantum-Well Heterostructure Lasers," J. of Appl. Phys. 52, 7201 (1981).

88. J. J. Coleman, P. D. Dapkus, M. D. Camras, N. Holonyak, Jr., W. D. Laidig, T. S. Low, M. S. Burroughs, and K. Hess, "Absorption, Stimulated Emission, and Clustering in AlAs-$Al_xGa_{1-x}As$-GaAs Superlattices," J. of Appl. Phys. 52, 7291 (1981).

89. N. Holonyak, Jr., W. D. Laidig, M. D. Camras, H. Morkoç, T. J. Drummond and K. Hess, "Clustering and Phonon Effects in $Al_xGa_{1-x}As$-GaAs Quantum-Well Heterostructure Lasers Grown by Molecular Beam Epitaxy," Solid State Commun. 40, 71 (1981).

90. K. Hess, "Lateral Transport in Superlattices," Proc. 3rd Int. Conf. on Hot Electrons, Montpellier France, 1981.

91. P. A. Martin, K. Hess, and B. G. Streetman, "Electric Field Enhanced Emission from Non-Coulombic Traps in Semiconductors," J. Appl. Phys. 52, 7409 (1981).

92. K. K. Mon and K. Hess, "Resonance Impact Ionization in Superlattices," Solid-State Electronics 25, 491 (1982).

93. M. S. Burroughs, K. Hess, N. Holonyak, Jr., W. D. Laidig and G. E. Stillman, "Alloy Clustering and its Effect on Impact Ionization in Ternary III-V Compounds," Solid State Electronics 25, 161 (1982).

94. M. Keever, T. J. Drummond, H. Morkoç, K. Hess, B. G. Streetman, and M. Ludowise, "Hall Effect and Mobility in Heterojunction Layers," Journal of Applied Physics 53, 1034 (1982).

95. N. Holonyak, Jr., B. A. Vojak, H. Morkoç, T. J. Drummond, and K. Hess, "Stimulated Emission in a Degenerately Doped GaAs Quantum Well," Appl. Phys. Lett. 40, 658 (1982).

96. A. Bhattacharyya, K. Hess, and B. G. Streetman, "Comments on the Plasma Annealing Model to Explain the Dynamics of Pulsed Laser Annealing of Ion-Implanted Silicon," J. Appl. Phys. 53, 1261 (1982).

97. K. Hess, J. Y. Tang, K. Brennan, H. Shichijo, and G. E. Stillman, "Reply to Comment on 'Simulation of High-Field Transport in GaAs Using a Monte Carlo Method and Pseudopotential Band Structures' and on 'Band-Structure Dependent Transport and Impact Ionization in GaAs'," J. Appl. Phys. 53, 3327 (1982).

98. Paul D. Coleman, J. Freeman, H. Morkoç, K. Hess, B. Streetman, and M. Keever, "Demonstration of a New Oscillator Based on Real-Space Transfer in Heterojunctions," Appl. Phys. Letters 40, 493 (1982).

99. K. Hess, "Aspects of High Field Transport in Semiconductor Heterolayers and Semiconductor Devices," in Advances in Electronics and Electron Physics, ed. by P. W. Hawkes, vol. 59, pp. 239-291, (New York: Academic Press, 1982).

100. S. W. Kirchoefer, N. Holonyak, Jr., K. Hess, D. A. Gulino, H. G. Drickamer, J. J. Coleman, and P. D. Dapkus, "Absorption Measurements at High Pressure on AlAs-$Al_xGa_{1-x}As$-GaAs Superlattices," Appl. Phys. Lett. 40, 821 (1982).

101. J. Y. Tang and K. Hess, "Investigation of Near Ballistic Transport Following High Energy Injection," IEEE Trans. on Electron Devices ED-29, 1906 (1982).

102. S. W. Kirchoefer, N. Holonyak, Jr., K. Hess, D. A. Gulino, H. G. Drickamer, J. J. Coleman, and P. D. Dapkus, "High Pressure Experiments on $Al_xGa_{1-x}As$-GaAs Quantum-Well Heterostructure Lasers," Solid State Communications 42, 633 (1982).

103. Otto F. Sankey, J. D. Dow, and K. Hess, "Theory of Resonant Scattering in Semiconductors Due to Impurity Central-Cell Potentials," Appl. Phys. Lett. 41, 664 (1982).

104. J. Y. Tang, K. Hess, N. Holonyak, Jr., J. J. Coleman, and P. D. Dapkus, "The Dynamics of Electron-Hole Collection in Quantum Well Heterostructures," J. Appl. Phys. 53, 6043 (1982).

105. J. P. Leburton and K. Hess, "Energy Diffusion Equation for an Electron Gas Interacting with Polar Optical Phonons," Phys. Rev. B 26, 5623 (1982).

106. M. D. Camras, N. Holonyak, Jr., K. Hess, J. J. Coleman, R. D. Burnham, and D. R. Scifres, "High Energy $Al_xGa_{1-x}As$ ($0 \leq x \leq 0.1$) Quantum-Well Heterostructure Laser Operation," Appl. Phys. Lett. 41, 317 (1982).

107. M. Keever, K. Hess, and M. Ludowise, "Fast Switching and Storage in GaAs-$Al_xGa_{1-x}As$ Heterojunction Layers," IEEE Electron Device Lett. EDL-3, 297 (1982).

108. K. Hess, "Electron Transport in Heterojunctions and Superlattices," Proc. of the 16th Intl. Conf. on the Physics of Semiconductors, 1982 (invited paper).

109. J. Dow, S. Y. Ren, and K. Hess, "Random Superstructures," Phys. Rev. B 25, 6218 (1982).

110. W. T. Jones, K. Hess, and G. J. Iafrate, "Hot electron diffusion in fine line semiconductor devices," Solid-State Electronics 25, 1017 (1982).

111. S. W. Kirchoefer, N. Holonyak, Jr., K. Hess, K. Meehan, D. A. Gulino, H. G. Drickamer, J. J. Coleman, and P. D. Dapkus, "High pressure measurements on $Al_xGa_{1-x}As$-GaAs ($x = 0.5$ and 1) superlattices and quantum-well heterostructure lasers," J. Appl. Phys. 53, 6037 (1982).

112. M. Keever, W. Kopp, T. J. Drummond, H. Morkoç, and K. Hess, "Current Transport in Modulation Doped $Al_xGa_{1-x}As$/GaAs Heterojunction Structures at Moderate Field Strengths," Jpn. J. Appl. Phys., to be published.

113. N. Holonyak, Jr. and K. Hess, "Quantum-Well Heterostructure Lasers," (to be published).

114. G. J. Iafrate and R. Malik, J. Y. Tang, and K. Hess, "Transient Transport and Transferred Electron Behavior in GaAs Under the Condition of High Energy Electron Injection," (to be published).

Name: Thomas J. Hanratty

Present Position: Professor of Chemical Engineering, University of Illinois, Urbana

Birthdate: November 9, 1926

Education: B.Ch.E., Villanova University, 1947
M.S., Ohio State University, 1950
Ph.D., Princeton University, 1953

Scholastic and Professional Honors:

Allan P. Colburn Award, American Institute of Chemical Engineers, 1957
Curtis W. McGraw Award, American Society for Engineering Education, 1963
William H. Walker Award, American Institute of Chemical Engineers, 1964
Professional Progress Award, American Institute of Chemical Engineers, 1967
Member, National Academy of Engineering, 1974
Honorary Doctorate Degree, Villanova University, 1979
Senior Research Award, American Society of Engineering Education, 1979
Member, U. S. National Committee on Theoretical and Applied Mechanics, 1979-

Current Research Activities:

Currently carries out research with a group of thirteen graduate students in Chemical Engineering in the areas of turbulence, two-phase flow, flow over wavy surfaces, interfacial instabilities, convective mass transfer and reactor design.

Professional Experience:

University of Illinois, 1953-59, Assistant Professor; 1958-63, Associate Professor; 1963-present, Full Professor
Brown University, 1962, Visiting Associate Professor
Shell Development, summer, 1954
Rohm and Haas, summer, 1951
Battelle Memorial Institute, 1948-50, Res. Eng.
Fischer and Porter Company, 1947-48, Dev. Eng.

Current Professional Activities:

Advisory Committee for Engineering Division Oak Ridge National Laboratory, Advisory Committee Princeton University Chemical Engineering Department, Peer Review Committee NAE, Accreditation Committee AIChE, Editorial Boards of Physico Chemical Hydrodynamics, Physics of Fluids, Reviews in Chemical Engineering, Scientific Committees for Ninth National Congress on TAM and 3rd International Symposium on Turbulent Shear Flow, Cochairman Two-Phase Flow Symposium at L.A. Meeting of AIChE, Study Group for 1983 IUTAM Symposium on Experimental Techniques for Two-Phase Flow, Search Committee for Editor of Physics of Fluids, Evaluation Committee for NRC Res. Assoc. Program.

Current Research Grants:

Office of Naval Research; Wall Turbulence Compliance Surface Drag Reduction; N00014-88-82-120324; 4/1/83-3/31/84

National Science Foundation; Two-phase Flow and Mass Transfer; NSFCPE 82-19065; 6/15/83-6/14/84

American Institute of Chemical Engineers; Design Equations for Two-phase Flow; 9/1/83-8/31/84

National Science Foundation; International Cooperative Science Grant for Studies of Anular Gas Liquid Flow; 9/1/83-8/31/84.

PUBLICATIONS OF THOMAS J. HANRATTY

(1) With John N. Pattison, John W. Clegg, and Alexis W. Lemmon, Jr., "Thermal Decomposition of Hydrazine Vapor in Silica Vessel," Ind. Eng. Chem. 43, 113 (1951).

(2) "Nature of Wall Heat Transfer Coefficient in Packed Bed," Chem. Eng. Sci. 3, 209 (1954).

(3) "Turbulent Exchange of Mass and Momentum with a Boundary," A.I.Ch.E. Journal 2, 359 (1956).

(4) "Heat Transfer Through a Homogeneous Isotropic Turbulent Field," A.I.Ch.E. Journal 2, 1, 42 (1956).

(5) With Abdemannan Bandukwala, "Fluidization and Sedimentation of Spherical Particles," A.I.Ch.E. Journal 3, 293 (1957).

(6) "Velocity Profile for Fully Developed Turbulent Flow in a Pipe," A.I.Ch.E. Journal, September (1958).

(7) "Note on the Analogy Between Momentum Transfer and Heat or Mass Transfer for a Homogeneous Isotropic Turbulent Field," A.I.Ch.E. Journal, December (1958).

(8) With George Latinen and Richard H. Wilhelm, "Turbulent Diffusion in Particulately Fluidized Beds of Particles," A.I.Ch.E. Journal 2, 3, 372 (1956).

(9) With James M. Engen, "Interaction Between a Turbulent Air Stream and a Moving Water Surface," A.I.Ch.E. Journal 3, 3, 299 (1957).

(10) With Edward M. Rosen and Robert L. Kabel, "Effect of Heat Transfer on Flow Fields at Low Reynolds Numbers in Vertical Tubes," Ind. Eng. Chem. 50, 815 (1958).

(11) With Duane L. Flint and Hisao Kada, "Point Source Turbulent Diffusion in a Pipe," A.I.Ch.E. Journal 6, 325 (1960).

(12) With George F. Scheele and Edward M. Rosen, "Effect of Natural Convection on Transition to Turbulence in Vertical Pipes," Canad. J. of Chem. Eng. 67, June 1960.

(13) With Hisao Kada, "Effect of Solids on Turbulence in a Fluid," A.I.Ch.E. Journal 6, 624 (1960).

(14) With Edward M. Rosen, "Use of Boundary Layer Theory to Predict the Effect of Heat Transfer on Flow Field in a Vertical Tube with a Constant Temperature Wall," A.I.Ch.E. Journal 7, 112 (1961).

(15) With Arnold Hershman, "Initiation of Roll Waves," A.I.Ch.E. Journal 7, 488 (1961).

(16) With Lembit U. Lilleleht, "Measurement of Interfacial Structure for Co-Current Air-Water Flow," J. Fluid Mech. 11, 65 (1961).

(17) With Lembit U. Lilleleht, "Relation of Interfacial Shear Stress to the Wave Height for Co-Current Air-Water Flow," A.I.Ch.E. Journal 7, 548 (1961).

(18) With L. Philip Reiss, "Measurement of Instantaneous Rates of Mass Transfer to a Small Sink on a Wall," A.I.Ch.E. Journal 8, 245 (1962).

(19) "Relation of Lifetime Distribution to Age Distribution," in Chem. Eng. Sci. 57, January 1962.

(20) With Robert E. Johnk, "Temperature Profiles for Turbulent Flow in a Pipe. I. The Fully Developed Heat Transfer Region," Chem. Eng. Sci. 17, 867 (1962).

(21) With Robert E. Johnk, "Temperature Profiles for Turbulent Flow in a Pipe. II. The Thermal Entrance Region," Chem. Eng. Sci. 17, 881 (1962).

(22) With George F. Scheele, "Effect of Natural Convection on Stability of Flow in a Vertical Pipe," J. Fluid Mech. 14, 244 (1962).

(23) With George F. Scheele, "Effect of Natural Convection Instabilities on Rates of Heat Transfer at Low Reynolds Numbers," A.I.Ch.E. Journal 9, 183 (1963).

(24) With P. Van Shaw and L. Philip Reiss, "Rates of Turbulent Transfer to a Pipe Wall in the Mass Transfer Entry Region," A.I.Ch.E. Journal 9, 362 (1963).

(25) With Sadao Tanimoto, "Fluid Temperature Fluctuations Accompanying Turbulent Heat Transfer in a Pipe," Chem. Eng. Sci. 18, 307 (1963).

(26) With Paul Van Shaw, "Fluctuations in the Local Rate of Turbulent Mass Transfer to a Pipe Wall," A.I.Ch.E. Journa 10, 475 (1964).

(27) With L. Philip Reiss, "An Experimental Study of the Unsteady Nature of the Viscous Sublayer," A.I.Ch.E. Journal 9, 154 (1963).

(28) With L. S. Cohen, "Generation of Waves in the Co-Current Flow of Air and Liquid," A.I.Ch.E. Journal 11, 138 (1965).

(29) With Glen F. Crum, "Dissipation of a Sheet of Heated Air in a Turbulent Flow," Applied Scientific Research A15, 177 (1966).

(30) With Leonard S. Cohen, "Height of a Liquid Film in a Horizontal Concurrent Gas-Liquid Flow," A.I.Ch.E. Journal 12, 290 (1966).

(31) With James E. Mitchell, "A Study of Turbulence at a Wall Using an Electrochemical Wall Shear Stress Meter," J. Fluid Mech. 26, 199-221 (1966).

(32) With Kenneth R. Jolls, "Transition to Turbulence for Flow Through a Dumped Bed of Spheres," Chem. Eng. Sci. 21, 1185 (1966).

(33) With D. E. Woodmansee, "Stability of the Interface for a Horizontal Air-Liquid Flow," Proceedings of the Conference on Two-Phase Flow, Exeter, England, 1965 (Category 3).

(34) "A Study of Turbulence Close to a Solid Wall," Physics of Fluids Supplement, 5126 (1967), (Category 3).

(35) With Jaimie S. Son, "Limiting Relation for the Eddy Diffusivity Close to a Wall," A.I.Ch.E. Journal 13, 689 (1967).

(36) With L. S. Cohen, "Effect of Waves at a Gas-Liquid Interface on a Turbulent Air Flow," J. Fluid Mech. 31, 467 (1968).

(37) With Kenneth R. Jolls, "Use of Electrochemical Techniques to Study Mass Transfer Rates and Local Skin Friction to a Sphere in a Dumped Bed," A.I.Ch.E. Journal 15, 199 (1969).

(38) With Harry G. Dimopoulos, "Velocity Gradients at the Wall for Flow Around a Cylinder," J. Fluid Mech. 33, 303 (1968).

(39) With Anastasius J. Karabelas, "Determination of the Direction of Surface Velocity Gradients in Three-Dimensional Boundary Layers," J. Fluid Mech. 34, 159 (1968).

(40) With Donald E. Woodmansee, "Base Film Over Which Roll Waves Propagate," A.I.Ch.E. Journal 15, 712 (1969).

(41) With Donald E. Woodmansee, "Mechanism for the Removal of Droplets From a Liquid Surface by a Parallel Air Flow," Chem. Eng. Sci. 24, 299-307 (1969).

(42) With David P. Siegwarth, "Computational and Experimental Study of the Effect of Secondary Flow on the Temperature Field and Primary Flow in a Heated Horizontal Tube," Int. J. Heat and Mass Transfer 13, 27 (1970).

(43) With David P. Siegwarth, T. C. Readal, and Ritchie D. Mikewell, "Effect of Secondary Flow on the Temperature Field and Primary Flow in a Heated Horizontal Tube," Int. J. Heat and Mass Transfer 12, 1535-1552 (1969).

(44) With Jaimie S. Son, "Numerical Solution for the Flow Around a Cylinder at Reynolds Numbers of 40, 200, and 500," J. Fluid Mech. 35, 369-386 (1969).

(45) With Jaime S. Son, "Velocity Gradients at the Wall for Flow Around a Cylinder at Reynolds Numbers from 5×10^3 to 10^5," J. Fluid Mech. 35, 353 (1969).

(46) With Kamalesh K. Sirkar, "The Limiting Behavior of the Transverse Turbulent Velocity Fluctuations Close to a Wall," Ind. and Eng. Chem. Fundamentals 8, 189 (1969).

(47) With Kamalesh K. Sirkar, "Relation of Turbulent Mass Transfer to a Wall at High Schmidt Numbers to the Velocity Field," J. Fluid Mech. 44, 589-603 (1970).

(48) With Kamalesh K. Sirkar, "Limiting Behavior of the Turbulent Transverse Velocity Component Close to a Wall," J. Fluid Mech. 44, 605 (1970).

(49) With Gilead Fortuna, "Use of Electrochemical Techniques to Study the Effect of Drag Reducing Polymers in Flow in the Viscous Sub-Layer," Chemical Eng. Prog. Symposium Series Volume 67, Symposium Drag Reduction, 90-92 (1971).

(50) "A Course in Fluid Dynamics," Chemical Engineering Education 3, 161 (1969).

(51) With T. H. Wegner and A. J. Karabelas, "Visual Studies of Flow in a Regular Array of Spheres," Chem. Eng. Sci. 26, 59 (1971).

(52) With A. J. Karabelas and T. H. Wegner, "Use of Asymptotic Relations to Correlate Mass Transfer Data in Packed Beds," Chem. Eng. Sci. 26, 1581-9 (1971).

(53) With Gilead Fortuna, "Frequency Response of the Boundary Layer on Wall Transfer Probes," Int. J. Heat Mass Transfer 14, 1499-1507 (1971).

(54) With A. J. Karabelas, "Finite Difference Solution for Three Dimensional Boundary Layers with Large Positive and Negative Crossflows," A.I.A.A. Journal 8, 1527-1532 (1971).

(55) With Severino Zanelli, "Effect of Entrainment on Roll Waves in Air-Liquid Flow," Chem. Eng. Sci., 28, 643 (1973).

(56) With Masayoshi Miya and D. E. Woodmansee, "A Model for Roll Waves in Gas-Liquid Flow," Chem. Eng. Sci. 26, 1915-31 (1971).

(57) With A. J. Karabelas, "Measurement of Small Pressure Differences in a Gas-Liquid Flow," Rev. of Scientific Instruments 42, 1629-32 (1971).

(58) With Young Yuel Kim, "Weak Quadratic Interactions of Two-Dimensional Waves," J. Fluid Mech. 50, 107-32 (1971).

(59) With Gilead Fortuna, "The Influence of Drag-Reducing Polymers on Turbulence in the Viscous Sub-Layer," J. Fluid Mech. 53, 575 (1972).

(60) With K. K. Sirkar, "The Use of Electrochemical Techniques to Study Turbulence Close to a Wall," Proceedings of Symposium on Turbulence Measurements in Liquids, Rolla, September 1969, pp. 43-50.

(61) With L. D. Eckelman and Gilead Fortuna, "Drag Reduction and the Wave Length of Flow-Oriented Wall Eddies," Nature Physical Science 236, 94-96 (1972).

(62) With L. D. Eckelman, "Interpretation of Measured Variations of the Eddy Conductivity," Int. J. Heat Mass Transfer 15, 2231 (1972).

(63) With A. J. Karabelas and T. H. Wegner, "Flow Pattern in a Close Packed Cubic Array of Spheres Near the Critical Reynolds Number," Chem. Eng. Sci. 28, 673 (1973).

(64) "The Use of Electrochemical Techniques to Study Flow Fields and Mass Transfer Rates," published in "Heat and Mass Transfer in Flows with Separated Regions," edited by Z. Zaric, Pergamon Press, 1972.

(65) With James L. Taylor, "Influence of Natural Convection on Mass Transfer Rate for the Electrolysis of Ferricyanide Ions," Electrochimica Acta,(acçepted).

(66) With Myon Ki Lee and L. D. Eckelman, "Identification of Turbulent Wall Eddies Through the Phase Relation of the Components of the Fluctuating Velocity Gradient," J. Fluid Mech., 66, 17-33 (1974).

(67) With William Henstock, "The Interfacial Drag and the Height of the Wall Layer in Annular Flow," AIChE Journal, 20, 990-1000 (1976).

(68) With Dudley A. Shaw, "Turbulent Mass Transfer Rates to a Wall for Large Schmidt Numbers," AIChE Journal, 23, 28-37 (1977).

(69) With Dudley A. Shaw, "Influence of Schmidt Number on the Fluctuations of Turbulent Mass Transfer to a Wall," AIChE Journal, 23, 160-169 (1977).

(70) With David F. Tatterson and John C. Dallman, "Drop Sizes in Annular Gas-Liquid Flows," AIChE Journal, 23, 68-76 (1977).

(71) With D.D. McCoy, "Rate of Deposition of Droplets in Annular Two-Phase Flow," Int. J. Multiphase Flow, 3, 319-331 (1977).

(72) With Daniel P. Zilker and Gerald W. Cook "Influence of the Amplitude of a Solid Wavy Wall on a Turbulent Flow. Part I. Non-Separated Flows," J. Fluid Mech., 82, 29 (1977).

(73) With C. A. Thorsness, "Turbulent Flow Over Wavy Surfaces," Symposium on Turbulent Shear Flows, Pennsylvania State University, April 1977.

(74) With G. A. McConaghy, "Influence of Drag Reducing Polymers on Turbulent Mass Transfer to a Pipe Wall," AIChE Journal, 23, 493-500 (1977).

(75) With L. G. Chorn and D. T. Hatziavramidis, "Turbulent Fluctuations in the Viscous Wall Region for Newtonian and Drag Reducing Fluids," The Physics of Fluids, 20, 5112-119 (1977).

(76) With C. B. Thorsness and P. E. Morrisroe, "A Comparison of Linear Theory With Measurements of the Variation of Shear Stress Along a Solid Wave", Chem. Eng. Sci., 33, 579-592 (1978).

(77) With D. T. Hatziavramidis, "The Representation of the Viscous Wall Region by a Regular Eddy Pattern," Journal of Fluid Mechanics, 95, 655-679 (1979).

(78) With J. C. Dallman and B. G. Jones, "Interpretation of Entrainment Measurements in Annular Gas-Liquid Flows," Two-Phase Momentum, Heat and Mass Transfer, edited by F. Durst, G. V. Tsiklauri, N. H. Afgan, Vol. 2, p. 681, Hemisphere Publishing, 1979.

(79) With D. D. McCoy, "Droplet Mixing and Deposition in a Turbulent Flow," Two-Phase Momentum, Heat and Mass Transfer, edited by F. Durst, G. V. Tsiklauri, N. H. Afgan, Vol. 1, p. 119, Hemisphere Publishing, 1979.

(80) With W. H. Henstock, "Gas Absorption by a Liquid Layer Flowing on the Wall of a Pipe," A.I.Ch.E. Journal, 25, 122-131 (1979).

(81) With D. P. Zilker, "Influence of the Amplitude of a Solid Wavy Wall on a Turbulent Flow. Part 2. Separated Flows," J. Fluid Mech., 90, 257-271 (1979).

(82) With C. B. Thorsness, "Stability of Dissolving or Depositing Surfaces," A.I.Ch.E. Journal, 25, 697-701 (1979).

(83) With C. B. Thorsness, "Mass Transfer Between a Flowing Fluid and a Solid Wavy Surface," A.I.Ch.E. Journal, 25, 686-697 (1979).

(84) "Stability of Surfaces that are Dissolving or Being Formed by Convective Diffusion, Annual Reviews of Fluid Mechanics, 13, 231-52 (1981).

(85) With Jay A. Campbell, "Measurement of Wall Shear Stress," to be published in book on "Fluid Mechanics Measurements," edited by Richard J. Goldstein

(86) With J. A. Campbell, "Influence of Turbulence Structure on Mass Transfer at a Solid Surface," Proceedings of the 2nd Symposium on Turbulent Shear Flows, London (1979).

(87) With J. H. A. Hogenes, "The Use of Multiple Wall Probes to Identify Coherent Flow Patterns in the Viscous Wall Region," J. Fluid Mech., 124, 363-390 (1982).

(88) With J. A. Campbell, "The Mechanism of Turbulent Mass Transfer at a Boundary," "Turbulent Shear Flows 3," Selected Papers from the Third International Symposium on Turbulent Shear Flows, The Univ. of California, Davis, Sept. 9-11, 1981, edited by L. J. S. Bradbury, F. Durst, B. E. Launder, F. W. Schmidt, J. H. Whitelaw, published by Springer-Verlag, Berlin (1982).

(89) With J. A. Campbell, "Mass Transfer Between a Turbulent Fluid and a Solid Boundary: Linear Theory," A.I.Ch.E. Journal, 28, 989-993.(1982).

(90) With J. A. Campbell, "Mechanism of Turbulent Mass Transfer at a Solid Boundary," A.I.Ch.E. Journal, 29, 221-229 (1983).

(91) With J. A. Campbell, "Turbulent Velocity Fluctuations that Control Mass Transfer to a Solid Boundary," A.I.Ch.E. Journal, 29, 215-221 (1983).

(92) With Miltiadis Hiskakis, "Combustion of Carbon Residue from Oil Shale Retorting," A.I.Ch.E. Journal, 21, 451-459 (1983).

Curriculum Vitae

Robert Maxwell McMeeking
2312 Barberry Drive
Champaign, IL 61820
217-351-8347

Born: May 22, 1950, Glasgow, Scotland

Citizenship: United Kingdom
Registered as U. S. Permanent Resident August 9, 1977

Education:

1972-1976 Brown University, Providence, Rhode Island

Degrees: M. Sc. (Engineering) - June 1974

Ph.D. (Engineering), with major in Solid Mechanics and Minors in Materials Science and Applied Mathematics - June 1977 (Thesis advisor - James R. Rice)

1968-1972 University of Glasgow, Glasgow, Scotland

Degree: B. Sc. (Engineering), with First Class Honours in Aeronautical and Mechanical Engineering and Naval Architecture - July 1972

Experience:

1982- Associate Professor, Department of Theoretical and Applied Mechanics, University of Illinois at Urbana-Champaign

1978-1982 Assistant Professor, Department of Theoretical and Applied Mechanics, University of Illinois at Urbana-Champaign

1976-1978 Acting Assistant Professor, Division of Applied Mechanics, Department of Mechanical Engineering, Stanford University

1973-1976 Research Assistant in the Division of Engineering, Brown University

1971 Research Assistant (Summer Appointment) in the Department of Mechanics and Mechanisms, Faculty of Engineering, University of Glasgow

Awards:

1972-1975 University of Glasgow, Gray, Law and Watt Scholarship

1972-1973 University Fellowship, Brown University

1972 University of Glasgow, Goudie, George Harvey and George Russel Prizes

Activities: Member of American Society of Mechanical Engineers, Sigma Xi, American Academy of Mechanics, AAAS, American Society for Testing and Materials

Computing Committee and Fracture Mechanics Committee of Applied Mechanics Division, ASME
Mathematical Methods Committee of Engineering Mechanics Division, ASCE
Committee E24.08 (Ductile Fracture), ASTM

Invited Participant: Euromech Conference on the Mechanics of Glaciers, Interlaken, Switzerland, September 1983.

NSF-Max Planck Institut Workshop on Transformation Toughening in Ceramics, Tegernsee, W. Germany, June 1981.

DARPA Materials Research Council Conference on Fracture, San Diego, CA, July 1980.

The Metals Society Conference on Micromechanisms of Crack Extension, Cambridge, England, March 1980.

UIUC Committees: Advisory Committee, Department of Theoretical and Applied Mechanics, 1981-present.

College of Engineering ad hoc sub-committee on Computer Aided Design and Manufacturing, 1980-81.

Consulting: IBM, E. Fishkill, N.Y. (Current)
as Member, Structural Analysis Review Board, Teledyne CAE, Toledo, OH (Current)

Naval Ordnance Station, Indian Head, MD (1977-79).

Publications of R. M. McMeeking

"Finite-Element Formulations for Problems of Large Elastic-Plastic Deformation," with J. R. Rice, Int. J. Solids Structures, 1975, 11, pp. 601-616.

"The Weight Function Method for Determining Stress Intensity Factors," with P. C. Paris and H. Tada, ASTM-STP 601, 1976, pp. 471-489.

"Finite Deformation Analysis of Crack Tip Opening in Elastic-Plastic Materials and Implications for Fracture Initiation," J. Mech. Phys. Solids, 25, 1977, pp. 357-381.

"Path Dependence of the J-Integral and the Role of J as a Parameter Characterizing the Near Tip Field," Flaw Growth and Fracture, ASTM STP 631, pp. 28-41, 1977.

"Blunting of a Plane Strain Crack Tip into a Shape with Vertices," Trans. A.S.M.E. (Series H. J. Engg. Mat. Tech.) 99, pp. 290-297, 1977.

"Stress and Deformation Analysis of Metal Forming Processes," with E. H. Lee and R. L. Mallett, in Numerical Modeling of Manufacturing - Processes, A.S.M.E., pp. 19-33, 1977.

"A Finite Element Analysis of a Circumferentially Notched Tensile Specimen," with D. K. Brown, Fracture 1977 (ed. D.M.R. Taplin), Vol. 3, pp. 507-513, 1977, University of Waterloo Press.

"Finite Element Metal Forming Analysis with Spacially Fixed Mesh," with K. A. Derbalian, E. H. Lee and R. L. Mallett, in Applications of Numerical Methods to Forming Processes, A.S.M.E. AMD-Vol. 28, pp, 39-48, 1978.

"On a Theory of Central Burst or Chevroning Defects in Drawing and Extrusion," with E. H. Lee, Trans., A.S.M.E., (Journal of Engineering for Industry) 100, 1978, pp. 386-387.

"On Single Test Methods for Determining J During Crack Growth," with S. J. Burns, Int. J. Fracture, 14, pp. R73-R76, 1978.

"On Criteria for J-Dominance of Crack Tip Fields in Large Scale Yielding," with D. M. Parks, ASTM-STP 668, 1979, pp. 175-194.

"Recent Finite Element Studies in Plasticity and Fracture Mechanics," with J. R. Rice, D. M. Parks and E. P. Sorensen, Computer Methods in Applied Mechanics and Engineering, 17/18, 1979, pp. 411-442.

"Stress and Deformation Analysis of Metal-Forming Processes," with E. H. Lee and R. L. Mallett, Metal Forming Plasticity, Proceedings of IUTAM Symposium (Ed. H. Lippmann), Tutzing, W. Germany, 1978, Springer-Verlag, pp. 177-189, 1979.

"Resolution of Unresolved Safety Issue-Reactor Vessel Toughness," with M.P. Gomez and D. M. Parks, Report WUTA 7972-04 to Sandia Laboratories, September 1979.

"Concerning Elastic and Plastic Components of Deformation," with E. H. Lee, International Journal of Solids and Structures, 17, 1980, pp. 715-722.

"Stress and Plane Strain Fields at the Tip of a Stationary Tensile Crack in a Creeping Material," with F. A. Leckie, International Journal of Fracture, 17, 1981, pp. 467-476.

"Some Effects of Inelastic Constitutive Models on Crack Tip Fields in Steady Quasistatic Growth," with D. M. Parks and P. S. Lam, Advances in Fracture Mechanics, Proceedings of the 5th International Congress on Fracture, Cannes, France, March 1981, Vol. 5, pp. 2607-2614.

"An Incremental Crack Growth Model for High Temperature Rupture in Metals," with F. A. Leckie, Advances in Fracture Mechanics, Proceedings of the 5th International Congress on Fracture, Cannes, France, March 1981, Vol. 2, pp. 699-704.

"The Generation of Residual Stresses in Metal-Forming Processes," with E. H. Lee, Residual Stress and Stress Relaxation, Proceedings of 28th Sagamore Army Materials Research Conference, Lake Placid, 1981 (ed. E. Kula and V. Weiss) Plenum, New York, pp. 315-330, 1982.

The Finite Strain Tension Torsion Test of a Thin Walled Tube of Elastic-Plastic Material," International Journal of Solids and Structures, 18, 1982, pp. 199-204.

"The Mechanics of Transformation Toughening in Brittle Materials," with A. G. Evans, Journal of the American Ceramic Society, 65, 1982, pp. 242-246.

"Near-Surface Flow in Glaciers Obeying Glen's Law," with R. E. Johnson, TAM Report No. 454, September 1982, submitted to Quarterly Journal of Mechanics and Applied Mathematics.

"Estimates of the J-integral for Elastic-Plastic Specimens in Large Scale Yielding," to appear in Trans. ASME (Series H, J. Engg. Mat. Tech.) 1983.

"Estimates for the Constitutive Moduli of Ductile Materials Containing a Small Volume Fraction of Voids or Inclusions," Mechanics of Materials (D. C. Drucker Anniversary Volume) (eds. G. A. Dvorak and R. T. Shield) Elsevier, Amsterdam, 1983, in press.

"Analyses of Steady Quasistatic Crack Growth in Plane Strain Tension in Elastic-Plastic Materials with Non-isotropic Hardening," with P. S. Lam, TAM Report, 1983.

CURRENT RESEARCH GRANTS

1. "The Mechanics of Ductile Rupture and Plasticity"
   National Science Foundation 10/15/82 - 4/14/85
   MEA 82-11018 $120,291
   P.I. R. M. McMeeking

2. "The Mechanics of Toughening Mechanisms in
   Brittle Materials" $104,942
   Office of Naval Research 9/1/81 - 12/31/83
   P.I. R. M. McMeeking