THE SUPERCOMPUTER FAMINE IN AMERICAN UNIVERSITIES

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ABSTRACT

There is a strong, broadly-based need for the acquisition of a supercomputer by the University of Illinois. More than 65 faculty members (representing over 100 researchers) in fifteen departments are included in this report. They have documented an incredible array of frontier science areas they can attack if a supercomputer is available locally. They stress that a supercomputer would greatly improve faculty recruitment, retainment, and morale. It would form a high tech center which would attract major new industrial and grant support to the University.

An example of the type of supercomputer needed is the CRAY X-MP. It is 30-50 times than our CYBER 175, with 288 times the fast memory. It could be networked to the more than 20 local VAX machines currently owned by individual research groups. The X-MP would be available in late 1983. The capital cost is about $15 million with a continuing cost of approximately $1 million/year. Funding would be obtained from a combination of state, federal, and industrial sources.

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I. Supercomputers

By "supercomputer" I mean the computer with the largest memory and the fastest CPU currently available commercially. At the moment (September 1982), the two major American supercomputers are the CRAY-1 and the CYBER 205. Such machines possess 1-4 million 64-bit words in the central memory with a relative capacity of more than 4 CDC 7600's (the equivalent of 6 CYBER 175's). [See Appendix B for rough conversion figures.]

The CRAY X-MP machine, which becomes available in one year, will yield a throughput increase of ~3-5 over the CRAY-1. It also offers a 10 gigabits/sec transfer rate to 32 million (64-bit) words of external solid state memory, in addition to the 4 million words in central memory. This would make it equivalent to 30-50 CYBER 175s. The above figures are used to "set the scale" for what universities should be thinking about in the next few years, and do not constitute an endorsement of any manufacturer.

The current distribution of supercomputers (Appendix A) virtually excludes American universities. As of mid-1982 there are ~ 50 supercomputers in the world. In this country the national DOE weapons labs have the largest concentrations of them. Lawrence Livermore National Laboratory (LLNL) and Los Alamos Scientific Laboratory (LASL) each have four CRAY-1's, or 1/5 of the world supply. Specialized scientific groups have access to CRAY's at National Centers, e.g. the National Center for Atmospheric Research (NCAR) and the Magnetic Fusion Energy Center (MFECC). Finally, a number of major corporations have acquired CRAY's, e.g. Bell Labs and Exxon. European scientific centers have also begun using supercomputers, e.g. the Max-Planck Insitute (MPI) for Physics and Astrophysics in Garching-bei-Munchen, West Germany.

The first arrival of supercomputers at American universities has occurred in the last year. Colorado State University and Purdue University have each bought a CYBER-205, while the University of Minnesota has obtained a CRAY-1. At least a dozen universities are presently considering whether to purchase supercomputers either individually or in regional groups.

II. Flight From the Universities

The drought of computing power in the universities over the last five years has resulted in a a major drain of highly talented researchers from the universities to the sites with supercomputers. I perceive two stages in this process: first, a flight to the weapons labs (LLNL and LASL), and second, a flight to foreign computing centers. Most of this section is anecdotal knowledge and represents my narrow sphere of expertise. I imagine similar stories can be told by others in different areas of research.

Much of the work in computational astrophysics has been done at LLNL and LASL during the last decade. Areas of numerical research include: supernovae, general relativity (black holes, neutron stars, gravitational waves, cosmology), nonspherical accretion onto compact objects, jet formation, star formation, and radiation astrophysics. Many scientists from universities who wanted to work on these frontier fields were forced to go to the national labs to gain access to the largest 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 became lab employees. Others remained consultants to the labs so they could do their computing while remaining in the universities.

More recently, computational astrophysicists have been going to MPI in Munich, West Germany to do their computing. This is because the MPI CRAY-1 is devoted to physics and astrophysics, not to weapons design. Even scientists employed at the weapons labs can often get more CRAY time for their astrophysics projects at MPI than they can at LLNL or LASL. In the last two years the following astrophysicists have spent extended visits at MPI: David Arnett (U. of Chicago), Peter Bodenheimer (U. of CA.- Santa Cruz), Dick Miller (U. of Chicago), Michael Newman (LASL), Michael Norman (Ph.D. from U. of CA. -

Davis), Larry Smarr (U. of IL.), and Paul Woodward (LLNL). A similar list exists for theoretical chemistry. There are about 100 visitors to MPI per year, of which ~ 20 are heavy CRAY users.

Currently, the Japanese are furiously publishing work in the area of numerical hydrodynamics. Their major fields of attack so far are protostars, stellar evolution, accretion onto compact objects, radio jets, and general relativity. They are limited by their currently available computers, but within one to two years supercomputers will come on-line. At that point it is highly likely that Japan and Germany (already on-line) will take over from the U.S. the scientific leadership in numerical astrophysics.

Besides the obvious loss of talent from the universities to the weapons labs and foreign institutions, what are the other costs American universities must pay for lacking supercomputers? The primary problem is that numerical science must be done in the "crash program" mode. A visit to a supercomputer site is limited in duration: typically a few days to a few months. Thus one is under great pressure to complete a project in a short period of time. This means long hours (100 hours per week is not uncommon), great fatigue, little time for thinking or literature searching, and no time to discuss the project with colleagues. Furthermore, there is not the diversity of colleagues to confer with that one has nurtured in one's university. In many cases, one can't even look at the output of the calculation until one has left the site. This is not good scientific methodology.

Clearly, it would be much better to have the supercomputer (or access to one) at the home institution of the scientist. Then he could spend all year in "compute, think, read, talk, recompute" mode. That is, he could do a calculation, produce output graphically, thoughtfully look through it, realize he needed different functions plotted, compare his work with previous efforts,

discuss his ideas with other American-based collegues, do an analytic side-calculation, understand more deeply what the physics is, and then decide what to compute next. He has access to a friendly and comfortable local computing system instead of having to learn an entirely new, foreign system in a few days' time. He has graduate students, secretaries, his own office and library, and a familiar circle of scientific colleagues to talk with. All of these factors are important for good scientific research. Finally, only the most hardy souls with the most forgiving families can socially, psychologically, and physiologically withstand the constraints imposed by computing sessions at distant supercomputer sites. Having supercomputers available to universities would bring many more top scientists into the numerical science revolution.

III. Frontier Science and Supercomputers

The above arguments do not pinpoint why supercomputers, rather than say many small computers, are essential in areas of frontier science. Perhaps the most succinct statement is that attributed to Edward Teller. "Teller's Rule" is that the most challenging frontier problems in science require at least 100 hours on the fastest computer available. As computers become faster, the knowledge gained on previous machines enables one to fruitfully attack the next level of complexity. Currently, there is virtually nowhere in the world where one could get this much CRAY time in a year as on off-site visitor.

One could make the argument that such problems could be attacked on small host computers attached to dedicated array processors. Indeed, fundamental work in quantum field theory and astrophysics has been done in this mode by some groups (e.g. the Cornell array processor users group). However, to date most computational astrophysicists prefer to have the large memory, high

speed, fast turnaround of a supercomputer. The point is that the scientist should be able to choose the tool which best enables him to do his science on his timescale. Currently the answer to this choice is being masked by the physical difficulty of gaining access to supercomputers. Let me turn to a few examples of the type of fundamental science that is currently being done on supercomputers. Again let me stress that I can only relate areas of research I have personal familiarity with. The Press NSF Report "Prospectus for Computational Physics," 1981, details many more areas. Also, some of this work is work that will have to be done on supercomputers to get a reliable answer, but which is currently forced to be done on lesser computers (e.g. CDC 7600 or CYBER 175) because of lack of access to supercomputers.

My set of examples are a list of ~ 60 scientists at the University of Illinois whom I have talked to about the desirability of obtaining a supercomputer at the University of Illinois. These are researchers who would either actively use the supercomputer or bring in associates who would. The one-line description of areas of potential supercomputer research is augmented by more detailed statements of research intent in Appendix C. The clear conclusion is that there is a tremendous breadth of areas represented at only one major university.

POTENTIAL SCIENTIFIC PROJECTS
University of Illinois
CRAY X-MP Facility
(as of 11/1/82)

Physics Department

* Richard Brown (Prof.) + 9 other faculty	- Experimental Particle Physics
* Haldan Cohn (Res. Asst. Prof.)	- Evolution of Stellar Systems
	- Magnetohydrodynamical Accretion
* John Dow (Prof.)	- Electronic Materials
* Hans Frauenfelder (Prof.)	- Dynamics of Biological Molecules
* John Kogut (Prof.)	- Solving Quantum Chromodynamics
* Barry Kunz (Prof).	- Quantum Chemistry of Solids
* Fred Lamb (Prof.)	- Radiation Hydrodynamics of Neutron Stars
* V.R. Pandharipande (Prof.)	- Quantum Liquids and Solids
* David Ravenhall (Prof.)	- Nuclear Structure and Scattering
* John Stack (Assoc. Prof.)	- Quantum Field Theory
* Michael Stone (Assist. Prof.)	- Simulating Quantum Field Theory
* H. W. Wyld (Prof.)	- Lattice Quantum Chromodynamics and Turbulence Simulation

Astronomy Department

* Joan Centrella (Post. Doc.)	- Large Scale Structure of the Universe
* Helene R. Dickel (Res. Assoc. Prof.)	- Radio Interferometric Spectral Line Analysis
	- Radiation Hydrodynamics of Molecular Cocoons
* John Gallagher (Prof.)	- Optical Astronomy Instrumentation
* Icko Iben (Prof.)	- Stellar Evolution
* Steven Langer (Res. Assoc.)	- Accretion Onto Neutron Stars
* Telemachos Mouschovias (Assoc. Prof.)	- Star Formation
* Larry Smarr (Assoc. Prof.)	- Numerical General Relativity
	- High Resolution Finite Differencing of Hydrodynamics
* Lewis Snyder (Prof.)	- Chemical Astrophysics
* James Truran (Prof.)	- Hydrodynamics of Novae
	- Nucleosynthesis Networks

Chemistry Department

* David Chandler (Prof.)	- Quantum Dynamics of Molecules
* Clifford Dykstra (Assist. Prof.)	- Electronic Structure Theory
* Douglas McDonald (Prof.)	- Intramolecular Dynamics of Molecules
* Donald Secrest (Prof.)	- Molecular Scattering Theory
+ Peter Wolynes (Assoc. Prof.)	- Monte Carlo and Renormalization Group in Quantum Chemistry
	- Simulation of Solitons in Polymers

Computer Sciences

+ Roy Campbell (Assoc. Prof.)	- Software Engineering
* Charles W. Gear (Prof.)	- Numerical Software
* William Kubitz (Assoc. Prof.)	- VLSI Design Automation
* Daniel Gajski (Assoc. Prof.)	- "
* David Kuck (Prof.)	- Supercomputer Software & Algorithm Development
* Ahmed Sameh (Prof.)	- "
* Paul Saylor (Assoc. Prof.)	- Iterative Solution of Large Systems of Linear Algebraic Equations
* Dan Slotnick (Prof.)	- Supercomputer Design & Application
* Daniel Watanabe (Assoc. Prof.)	- Simulation of Semiconductor Devices

Atmospheric Sciences

* Stan Kidder (Assist. Prof.)	- Forecasting with Satellite Data
+ Yoshimitsu Ogura (Prof.)	- Simulation of Convection & Turbulence
+ Su-Tzai Soong (Assoc. Prof.)	- Simulation of Mesoscale Convection Systems
+ Kevin Trenberth (Prof.)	- Climate Modeling
+ John Walsh (Assoc. Prof.)	- Sea Ice Modeling
* Robert Wilhelmson (Assoc. Prof.)	- Dynamics of Severe Storms

Chemical Engineering

* Thomas Hanratty (Prof.)	- Turbulence
* Mark Stadtherr (Assoc. Prof.)	- Chemical Process Design

Electrical Engineering

* Jacob Abraham (Assoc. Prof.)	- VLSI System Design
* Sid Bowhill (Prof.)	- Three-Dimensional Atmospheric Modeling
* Edward Davidson (Prof.)	- Computer Architecture & Reliability
* Karl Hess (Prof.)	- Simulation of 3-D Submicron Semiconductor Devices
* Nick Holonyak (Prof.)	- Quantum-well Heterostructures
* W. Kenneth Jenkins (Assoc. Prof.)	- Inverse Problems in Tomography, Synthetic Aperture Radar Images, and Sonar Beam Forming
* Michael Pursley (Prof.)	- Performance Evaluation of Communication Systems
* Timothy Trick (Prof.)	- Two-Dimensional Simulation of Electronic Devices

Mechanical and Industrial Engineering

+ A. L. Addy (Prof.)	- Gas Dynamics
+ Richard Buckius (Assoc. Prof.)	- Radiation Heat Transfer
* Herman Krier (Prof.)	- Hydrodynamic Shock Physics
* Frederick Leckie (Prof.)	- Damage Mechanics

Theoretical & Applied Mechanics

+ Ronald Adrian (Prof.)	- Comparison of Simulated Turbulence with Experiment
* Lawrence Bergman (Assist. Prof.)	- System Dynamics
* Robert McMeeking (Assoc. Prof.)	- Fracture Mechanics

Civil Engineering

* Robert Haber (Assist. Prof.)	- Structural Optimization
* Leonard Lopez (Prof.)	- Structural Mechanics and CAD/CAM

Aeronautical & Astronautical Engineering	
* S. M. Yen (Prof.)	- Rarefied Gas Dynamics - Computational Fluid Dynamics
Anatomical Sciences	
* Jay Mittenthal (Assist. Prof.)	- Biomechanics of Cell Sheets
Genetics and Development	
* Robert Futrelle (Research Scientist)	- Simulation of Living Cells
Physiology and Biophysics	
* Eric Jakobsson (Assoc. Prof.)	- Emergent Oscillatory Properties of Neural Networks
Accountancy	
* James McKeown (Prof.)	- Multiple Time Series Analysis

* = spoken to by L. Smarr
+ = spoken for by * people

OTHER SUPERCOMPUTERS IN THE WORLD

Taken from the LAX Report: "Report of the Panel on Large Scale Computing in Science and Engineering," September 1982.

Partial Inventory and Announced Orders of Class VI Machines

Country	Site	Number	Purpose	Computer
U.S.	LANL	4	Weapons Research	Cray-1
	LLNL	4	Weapons Research	Cray-1
		2	MFE	Cray-1
	Sandia	2	Weapons Research	Cray-1
	KAPL	1	Reactor Research	Cyber 205
	Bettis	1	Reactor Research	Cyber 205
	Kirtland	1	Military	Cray-1
	NCAR	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
	Colorado State	1	Engineering Research	Cyber 205
	Minnesota	1	Research	Cray-1
	Princeton GFDL	2	Geophysics	Cyber 205
	Purdue	1	Research	Cyber 205
	Georgia	1	Research	Denelcor HEP
	CHEVRON	1	Petroleum	Cray-1
	Bell	1	Research	Cray-1
	ARCO	1	Petroleum Engineering	Cray-1
	EXXON	1	Petroleum Engineering	Cray-1
	TEXACO	1	Petroleum Engineering	Cyber 205
	SOHIO	1	Petroleum Engineering	Cyber 205
	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
France	GETIA	1	Electric Power Inst.	Cray-1
England	ECMWF	1	Weather	Cray-1
	Brit Met	1	Weather	Cyber 205
	Daresbury	1	Physics Research	Cray-1
	AWRE Harwell	1	Nuclear Energy, Weapons	Cray-1
	Shell Oil, U.K.	1	Petroleum	Cray-1
	Univ. of London	1	Research	Cray-1
Japan	Mitsubishi	1	Research	Cray-1
	Century Research	1	Research	Cray-1

APPENDIX B

COMPUTER EQUIVALENCE TABLE

Taken from the Press Report: "Prospectus for Computational Physics," 1981

COMPUTER EQUIVALENCE TABLE*

Manufacturer	*Model*	*Relative Capacity*	*Nominal Capacity NSU's)*
CRI	CRAY-1	4.0	40,000
CDC	STAR-100	1.8	18,000
CDC	7600	1.0	10,000
IBM	3033	.95	9,500
IBM	360/370/195	.95	9,500
UNI	1100/82	.88	8,800
UNI	1100/44	.88	8,800
CDC	CYBER 175	.70	7,000
IBM	360/168-3	.58	5,800
IBM	370/168-1	.53	5,300
IBM	360/91	.51	5,100
UNI	1108	.29'	2,900
IBM	3031	.24	2,400
CDC	6600	.22	2,200
CDC	CYBER 174	.22	2,200
IBM	370/158	.20	2,000
IBM	360/75	.20	2,000
CDC	CYBER 74	.18	1,800
IBM	IBM 360/65	.16	1,600
DEC	PDP KL10	.14	1,400
CDC	CYBER 73	.12	1,200
DEC	VAX 11/780	.12	1,200
CDC	6400	.11	1,100
HIS	66/40	.11	1,100
IBM	360/44	.07	700
DEC	PDP KI10	.06	600
DEC	PDP KA10	.04	400
IBM	360/50	.036	360
DEC	11/70	.036	360
DEC	11/45	.033	330

'Specifically UNI 1108 complex at SLA.

*SOURCE: Department of Energy FY 1981-1985 ADP Long Range Plan

APPENDIX C

SCIENTIFIC OPPORTUNITIES

Included herein are short statements of important new scientific problems that could be attacked at Illinois with a supercomputer. They were written and submitted to me by the faculty members named.

PHYSICS DEPARTMENT

Experimental Particle Physics (R.M. Brown)

The Experimental Particle Physics Group currently uses approximately 1000 hours per year of CYBER 175 CPU time equivalent 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; the Monte Carlo calculations are predominantly compute-bound. This work is being accomplished on facilities available through experiment collaborators at national laboratories (SLAC and FNAL). The Group's dedicated facility on-campus is principally used for equipment design, small sample data analysis, and program development.

On a supercomputer such as the CRAY X-MP, our data reduction needs require the heavy use of data tapes; on the other hand, the capability of such a machine for computation-intensive research calculations would be highly valuable. In particular, design and modeling of new massive experimental detectors requiring extensive CPU time would be possible with faculty and graduate students in residence at UICU. 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.)

Evolution of Stellar Systems (H. Cohn)

The evolution of dense multi-species stellar systems (e.g. galaxy clusters containing a wide range of galaxy masses, and galactic nuclei containing a range of stellar masses) is described by the multi-species collisional Boltzmann equation. The detailed models produced by the integration of this equation will be invaluable in interpreting high angular resolution Space Telescope observations of dense stellar systems. The present computational facilities at Illinois do not permit a treatment of the full multi-species collisional Boltzmann equation.

Magnetohydrodynamical Accretion (H. Cohn)

Implicit methods for analyzing accretion flows onto compact objects (e.g. disk accretion by a magnetized neutron star) present several advantages over the usual explicit schemes for studying such systems in which the evolution timescale significantly exceeds the dynamical timescale. Present computational facilities at Illinois are not adequate for an implicit treatment of a time dependent two-dimensional MHD system.

Physics of Biomolecules (H. Frauenfelder)

Computers are essential for the exploration of the physics of biomolecules. Biomolecules are complex, but extremely well designed many-body systems. We can expect that the deeper understanding of the physics of biomolecules will be of great interest not only to physics, but also to chemistry, biology, medicine, and pharmacology. Even very large present-day computers are barely adequate in at least three areas of biomolecular physics:

(1) Molecular dynamics calculations. Such computations, pioneered by Karplus and collaborators, are severely limited by the capabilities of present-day systems. A supercomputer would extend the range of calculations in two important directions -- towards more complex systems and towards longer times.
(2) Computer evaluation of X-ray diffraction data. X-ray diffraction, pioneered by Perutz and Kendrew, has played a crucial role in the elucidation of the structure of biomolecules. Recent work, started here at the UI in collaboration with Petsko at MIT, has shown that X-ray diffraction can yield far more information than just the static structure. It is to be expected that the extension of the new approaches, particularly when combined with synchrotron radiation and cryogenics, will place even more demands on computer capabilities.
(3) Simulation of protein action. The complexity of proteins renders the computer evaluation and description of protein phenomena much more complex than those of, for instance solids.

Large-Scale Computer Simulations of Elementary Particle Physics (J. Kogut)

Recent developments in high energy physics indicate that the fundamental particles, their properties and interactions can finally be studied theoretically by systematic numerical methods. The breakthroughs in this field have consisted of the realization that gauge theories describe the particles and their interactions, and that these theories can be solved approximately using discrete methods (lattice gauge theory). A major effort by the high energy theorists of our physics department has yielded significant results in this field. Computer simulations have produced good estimates of the masses of elementary particles, properties of nuclear matter, the behavior of scattering amplitudes, etc. These "first principles" calculations lie at the heart of both elementary particle and nuclear physics. Computer simulations in this field require the largest, fastest machines available. A typical simulation must manipulate at least 1-10 million real variables. Relaxation and Monte Carlo procedures require considerable computer time -- hundreds of CDC-7600 CPU hours are necessary for even the simplest, respectable calculation. Supercomputers are essential to continue and improve these research efforts.

Quantum Chemistry of Surfaces (A.B. Kunz)

Research in the area of quantum chemistry of surfaces and chemisorption and the optical properties of solids now requires precision of theoretical models of the order of 0.1 eV or better if one is to make either predictions of industrial use or test competing theoretical models which purport to explain observed phenomena. We are heavily involved in extending the horizons of existing models such as the Hartree-Fock model by direct incorporation of many-body effects by methods of configuration interaction and by use of many-body perturbation theory. In the case of configuration interaction methods, we

need the ability to find all the eigenvalues and eigenvectors of large matrices ($10^3 \times 10^3$) rapidly and accurately. In this instance the matricies in question are dense. In a few years the state of the art should be to couple molecular dynamic techniques with highly accurate quantum chemical computation of atomic interactions in order to predict all manner of surface processes. Currently, I have no access to any existing supercomputer and my research has been curtained by this. My hardware needs include reasonable, large, fast disc storage $\sim 6 \times 10^8$ bytes, large core memory $1 \times 10^6 + 4 \times 10^6$ words and high speed processing.

Accretion by Degenerate Stars (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. The study of those flows requires numerical integration of coupled two- or three-dimensional partial differential equations describing both the magnetofluid dynamics and the radiation field, under extreme conditions (temperature $\sim 10^{12}$ K, magnetic fields $\sim 10^{12}$ G, velocity approaching the speed of light, and enormous radiation energy densities). With our current computing facilities, only idealized one-dimensional and some two-dimensional calculations have been attempted. With a supercomputer, Illinois faculty could become pioneers in solving these problems.

Quantum Liquids and Solids (V.R. Pandharipande)

There is now a significant move in the microscopic theory of nuclei, and quantum liquids/solids in general, to use the Monte Carlo method (variational and Green's function) to study properties of interest. It appears that similar methods are useful to study chemical bonds, mesons and hadrons as few quark systems, etc. Most of the Monte Carlo work of my group is in collaboration with Argonne National Lab (which has a network of IBM 370/195 and two 3033's) and Ruhr Universitat Bochum (CYBER 205). It has been impractical to do the calculations in Urbana; our current use is ~ 500 CYBER 175 hours/year. Such collaborations are useful and will continue, but our inability to share any significant burden of computing will eventually go against us. Secondly I believe the collaboration will be more useful to the UI faculty if we could use a local supercomputer. I believe that there are many others on our faculty in my situation. Our research programs would become restricted if we do not have a supercomputer like CYBER 205 or CRAY X-MP quite soon.

Nuclear Structure and Scattering (D.G. Ravenhall)

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

(1) Nuclei reactions induced by electrons, and multiphoton corrections to the usual one-exchanged-proton approximation, involve the coupling together of several nuclear energy levels. The degree to which the calculation can approach reality is limited by the size of the storage available. The largest calculations performed with this program were done away from Illinois because of size and time limitation. That research program is in abeyance because of the size limitation, to some extent.

(2) Nuclear structure calculations using the random-phase approximation become more realistic the more excited nuclear configurations that can be included. Work with J. P. Blaizot here last semester was very much hindered by the 138 K storage limitation of the CYBER. This program is one we hope to continue, in collaboration with nuclear experimenters.

Simulation of Turbulence (H.W. Wyld)

An important and interesting field in which supercomputers will play a decisive role is the simulation of chaotic phenomena such as turbulence. There are a number of subdivisions in this area of research, ranging from the new and rapidly growing area of studies of chaotic phenomena in recursive maps and differential equations as models for the onset of turbulence, through engineering applications, to studies of so-called fully developed turbulence.

The general problem of fully developed turbulence was formulated many years ago. The nonlinear terms in the Navier-Stokes equations cause migration of long wavelength energy to smaller and smaller wavelengths, i.e. smaller and smaller eddies, until it reaches a very small wavelength where it is dissipated in heat through the viscosity terms. Despite many attempts over the years to describe this process analytically, the problem has not been solved or understood in any detail.

The best approach to the problem would seem to be numerical simulation on a large computer. There have, of course, been many numerical studies over the years [e.g. work by Orszag (MIT) and Siggia (Cornell) on CRAY-1]. All such attempts have been more or less frustrated by inadequate computers. Definitive studies of the problem require supercomputers which are both faster and have larger memories.

ASTRONOMY DEPARTMENT

The Large Scale Structure of the Universe (J. Centrella)

The recent evidence for nonzero neutrino rest masses has led many cosmologists to consider the effects of such particles on the formation of structure in the universe. The natural scale which emerges from the collisionless damping of heavy neutrino perturbations is $\sim 10^{15}\ M_0$, a supercluster mass. Centrella and Melott (Pittsburgh) are studying this large scale structure of the universe using a three-dimensional cloud-in-cell code to follow the gravitational interaction of massive neutrinos. They find that a cellular structure of interacting supercluster pancakes forms; this cellular structure has also been seen in two-dimensional simulations and in observations of the galaxy distribution on large scales. Using the CRAY-1 computers at Livermore they have run a model on a 32 x 32 x 32 mesh with 27 clouds per cell; such a large number of clouds is crucial to avoid spurious lumpiness and to get an accurate picture of the morphology of these large scale systems. A further simulation on a 64 x 64 x 64 mesh will provide better resolution of these structures and is planned for late 1982. The data from this project are being analyzed using the graphics facilities of the image processing center in the Astronomy building. Both finer meshes and more frequent runs are needed. These could be achieved at Illinois if we had a supercomputer.

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 10^8 integrations using the full VLA (351 individual interferometer

pairs), 256 frequency-channels to produce 256 full resolution maps of 2000 by 2000 grid points (4×10^6 data 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 30^s integrations with $1/4$ the possible interferometer pairs, $1/4$ 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" 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.

Hydrodynamical and Radiative Transfer Calculations 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 full CDC 7600 computer. In addition, the radiative tranfser effects in such a clumpy medium are being explored by means of a slightly modified version of the KPNO (#555) 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, it would also allow development of a more realistic, 3-dimensional treatment.

New Astronomical Instrumentation (J.S. Gallagher)

The availability of high capacity computer systems to observational astronomers may well be a necessity if full advantage is to be made of projected instrumental capabilities. Consider a two-dimensional Fourier transform spectrometer which is currently under development. This will allow moderate to high resolution spectra to be obtained over an image which eventually should have considerable size (~ several hundred pixels square). The data will then consist of the Fourier transform of the spectrum as observed by each pixel in the detector, i.e. typically $10^4 - 10^5$ spectra per object per observation set. Clearly extensive operation of such an instrument will depend on large computers, but the results, narrow band images of astronomical objects, will be critical in understanding energetic processes, for example, in sites of ongoing star formation.

Stellar Image Analysis (J.S. Gallagher)

Data analysis can be a real problem. A good illustration is provided by the difficulties associated with determining brightness of stars in crowded areas where the individual star images overlap (as in most interesting extragalactic systems). It is then necessary to fit and subtract the surroundings of each star with a complex background function and determine the brightness of each target star by some optimal chosen fit of the instrument response pattern to the star. Usually one would like to do this for minimally several 100 stellar objects which can be detected in $\leq$ 1 hr. with a modern detector or moderate to large telescopes. Such large data set processing on human scientific research timescales requires very large computers.

Stellar Evolution (I. Iben, Jr.)

To properly study the now low mass stars on the asymptotic giant branch (which is the last "quiescent" phase preceding the white dwarf or supernova phase) construct and bring to the surface carbon and neutron-rich isotopes, one needs to evolve perhaps a dozen model stars (of different initial masses and compositions) through approximately 20 thermal pulses. Such an operation requires ~ 128K memory and ~ 12 x 300 hours on a CYBER 175 (= 6-12 years work in real time). The same job could be done in ~ 70 hours on a CRAY X-MP (2 months in real time).

Radiation Hydrodynamics in Strong Magnetic and Gravitational Fields (S. Langer)

I am developing theoretical models of accreting neutron stars and white dwarf stars, particularly studying the effects of enormous magnetic fields and radiation pressure. These models require the numerical solution of the hydrodynamic equations to obtain the temperature and density structure in the flow and the equations of radiative transfer to obtain the spectrum of the emergent radiation. A simplified one-dimensional model already uses large amounts of CYBER 175 time. A realistic solution requires solving the coupled two-space dimensional equations. This would require must more fast memory than is available on the CYBER 175. The time-dependent, one-dimensional model for accretion onto white dwarf stars that is currently in use already consumes a significant amount of computer time. A full model of the type indicated above would require large amounts of time and considerably more memory than is available on the CYBER 175.

I am currently running models on the CRAY-1 computer at NCAR in an attempt to get around the limitations of the CYBER 175. This solution is not particularly satisfactory because of the long turnaround for obtaining hard-copy output and because the NCAR system is not oriented toward the development of new models. Attempts to develop models on the CYBER 175 and then make production runs at NCAR are not effective becuase of software incompatibilities between the two systems and the length of time even a test run requires. A supercomputer at UI would allow progress on these models to proceed in a timely fashion.

Star Formation (T. Ch. Mouschovias)

Availability on campus of a supercomputer can (1) render problems feasible in interstellar gas dynamics and star formation which are now only distant

dreams; (2) appreciably shorten the length of real time over which projects under way in the above areas can be completed; and (3) serve as a powerful gambit to attract bright young astrophysicists (theorists and observers) who need and rely increasingly more heavily on powerful supercomputers for their research aimed at the formulation of a theory of star formation.

High Resolution Gas Dynamics (L. L. Smarr)

The large memory and high speed of supercomputers allows one to simulate dynamic gas flows with high resolution. Astrophysical examples are the flows that occur in quasars and radio galaxies. These can involve the central powerhouse of active galactic nuclei - nonspherical accretion onto supermassive black holes [J. Hawley and L. Smarr (Univ. of Ill.) with J. R. Wilson (LLNL) - calculations performed on CRAY-1 at LLNL]. Or they can involve the formation, propagation, and stability of supersonic and relativistic jets in these objects [calculations by MUNAC (Munich Numerical Astrophysics Coalition) - M. Norman (MPI), K.-H. Winkler (MPI) and L. Smarr (Univ. of Ill.) on the MPI CRAY-1 and by J. R. Wilson (LLNL) on the LLNL 7600]. The use of large numbers of grid points ($\sim 5 \times 10^4$) allow theoretical resolution of the flows comparable to the observational resolution of the Very Large Array of radio telescopes or the Einstein orbiting x-ray telescope.

Numerical Relativity (L. L. Smarr)

Here one solves the fully time-dependent Einstein equations of general relativity to study the strongly curved spacetime near black holes or in the early universe. Again, many grid points ($>10^4$) are needed to cover both regions near the strong gravitational field as well as far away. Recent projects computed include formation of nonspherical black holes and neutron stars, generation of gravitational waves, and distribution of the dark matter in the universe [J. Centrella (Univ. of Ill.), L. Smarr (Univ. of Ill.), P. Dykema (LLNL), C. Evans (Univ. of Texas), and J. R. Wilson (LLNL) - calculations on LLNL CRAY-1]. Detailed calculations of these nonlinear processes are needed by the experimentalists designing gravitational wave detectors.

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 sustems 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 dimensional calculations are appropriate in this case. Here again there is a demand for greater computing power than is currently available here 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 computation facilities than are currently available at Illinois, and thus progress in this area is now being realized at other research centers.

CHEMISTRY DEPARTMENT

Theoretical Chemistry (D. Chandler and P. G. Wolynes)

One of the frontiers of modern physical chemistry is the understanding of quantum dynamics of molecules in many body systems. At Illinois, these problems are being attacked on several fronts. The path integral approach to quantum mechanics, when combined with modern statistical mechanical theory provides a powerful and multifaceted tool for studying various phenomena:

1). Chemical Kinetics. All electron transfer and proton transfer reactions involve tunneling in condensed phases. Tunneling also plays a role in cryogenic chemical reactions.

2). Localization Phenomena. The dynamics and structural features associated with electronic and vibrational excitations in liquids and other amorphous materials play a central role in condensed phase physical, chemical and biological processes, including photosynthesis.

The path integral approaches to these problems can be most profitably carried out through numerical methods that require large computational facilities. Among these methods are Monte Carlo techniques often utilizing analytical results to improve the requisite importance sampling. This makes possible the treatment of the many fermion aspects of chemical bonding and the complications of real time dynamics inherent in rate phenomena. Another technique intensive in computer time is the use of renormalization group calculations of the structure of localized states in condensed phases. Both of these approaches are facilitated by array or pipeline architecture.

Electronic Structure Theory (C. E. Dykstra)

The study of essentially all problems of structure and energetics in chemistry can be done, in principle, by theoretical treatments. The general approach is to solve for the electronic structure of a molecular species and thereby map out its energetics with respect to molecular distortions or even reactions. The difficulty has been in the quantitative incorporation of important electron correlation effects when solving for electronic structures. These many-body effects are the consequence of instantaneous electron-electron interactions. In recent years, the electron correlation problem has almost

become a solved problem because of methodological developments, including certain powerful electron pair operator techniques developed and implemented here at Illinois. We have calculated molecular structures to an accuracy of about 0.001 Å, identified a new molecule on the basis of our computation of its energetic stability, and obtained precise spectroscopic parameters for chemically bound molecules as well as certain transient species. What has not yet been accomplished with these theoretical electronic structure calculations is the study of large molecular systems, because the number of operations at comparable accuracy increases as the fourth, fifth or sixth power of the number of electrons. The computation of a simple reaction of two ethylene molecules can be 20 times as expensive to study as the properties of one ethylene molecule. Multiple or array processors can cut the dependence on the number of electrons considerably, and groups at NASA-Ames, Sandia and Los Alamos are currently using supercomputers to produce results which far outweight our restricted, standard-computer methods. This is especially unfortunate because coefficient matrix techniques, which we are responsible for, appear to be most suited for supercomputers or multiple processors. Were one of these machines available we would not only recover the advantage in this field but would go even farther ahead.

Intramolecular Dynamics Calculations (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 classical 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 (Univ. of Ill.)]. This remains the only work with a statistically significant number of trajectories. What is really needed are quantum calculations on intramolecular energy transfer. These calculations are completely hopeless without the latest generation supercomputers. Even on these computers they count as large scale work.

Molecular Scattering Theory (D. Secrest)

Most of the interesting results in scattering theory at present are based on approximations of questionable validity. The reason for this is that while techniques exist for solving these problems exactly, 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. 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. Thus essentially nothing is known about these processes. Crude model calculations have shown that the approximations do not work, but extensive accurate calculations must be made before there is any hope of solving these problems. 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.

COMPUTER SCIENCE

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 hierarchical 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 extremely 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.

Supercomputer Software and Algorithm Development (D.J. Kuck and A. Sameh)

This group studies compilers (Kuck) and algorithms (Sameh) especially aimed at supercomputers. The CRAY X-MP is particularly interesting because it has both a vector nature (as in the CRAY-1) and a multiprocessor nature (2 processors). Having a CRAY X-MP on the campus would allow us to experiment directly with the machine instead of obtaining small amounts of time at remote sites. Since the X-MP is capable of supporting more than two processors, the configuration could be expanded in the future to meet expanding needs.

Scientific Processors and 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 parallel 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.

Semiconductor Device Simulation (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. A supercomputer such as the CRAY would greatly facilitate this work because our current computing resources are barely adequate for such computation 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.

ATMOSPHERIC SCIENCES

Forecasting with Satellite Data (S. Kidder)

The best scheme for short-term (0-3 hr) weather forcasts is often simply extrapolation of current conditions. A potentially interesting way to achieve this is to use past and current satellite images to forecast the satellite picture a few hours ahead. This could be particularly valuable for fog forecasts and the movement of precipitation areas. The difficulty which one encounters is that satellite images have been described as having high volume-low information density data. A 1 km resolution visible GOES images of Illinois, for example, contains about 10^6 pixels (bytes) of information. To be useful, a forecast image must contain a similar number of pixels, and at least two past images are required to make each forecast. A large, fast computer, therefore, is required to contain all of the data and to process them in a timely fashion. Preliminary experiments on the CRAY-1 at NCAR indicate that such a forecast is possible, though much more research will be necessary before an accurate scheme can be developed.

Modeling the Interaction between Clouds and the Larger Scale Environment (S.-T. Soong)

We have been working on the problem of cloud initiative, structure and cloud cluster properties using a numerical cloud cluster model during the past several years. The purpose of this work is to identify the conditions for cloud formation and factors controlling the life-cycle of a cloud cluster. The ultimate goal is to improve the accuracy of precipitation forecasts. This kind of model requires a grid interval small enough to resolve individual clouds and a domain size large enough to contain the entire area of the cloud cluster as well as its nearby large-scale environment. The available computer time memory restricted our use of the model to two-dimensions (x-z). Recent studies have indicated that the three dimensional flow structure may be instrumental in the determination of the structure and precipitation characteristics of cloud clusters.

We are now extending our research efforts into the evolution of large-scale circulations and their embedded precipitation systems by acquiring a nested grid model developed at the National Meteorological Center. This will allow resolution of interesting mesoscale features, such as fronts and precipitation areas. Computer memory and computer time again dictate the grid resolution which can be used in such a model covering half the earth's atmosphere.

In our longer range planning, we intend to study cloud cluster properties with a full three-dimensional model for an area of a few hundred kilometers. This model has already been formulated but cannot be run for its intended purpose due to computer limitations. Our ultimate desire is to mesh the cloud cluster model with the nested grid model to complete the study of interaction between clouds and large-scale environments. This study would not be possible without a more powerful computer.

Climate Modeling (K. Trenberth)

Experiments are planned with a climate model. Such a model incorporates a full three dimensional simulation of the atmosphere and is 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.

At present these plans are tenuous but could be carried out, for example, at the NCAR on the CRAY-1A machine there. However, the extensive need for post-processing software would make this work much easier at the University of Illinois.

Sea Ice Modeling (J. Walsh)

The extent of sea ice is observed to vary by 100-1000 km on an interannual basis. Speculative arguments and empirical analyses suggest that these fluctuations may play a role in short-term climatic variations over large portions of the Northern Hemisphere. A two-dimensional viscous-plastic sea ice model is being used in our NSF-supported project to perform multiyear (10-20 year) simulations of arctic sea ice thickness and extent. With a partitioning of the ice thicknesses into the minimal two categories (less than, greater than 0.5 m), a 10-year simulation requires 1 $\frac{1}{2}$ hours of CPU time on the NCAR CRAY-1. However, a more realistic treatment of dynamical processes within the pack requires a more detailed resolution of the categories of thin ice to which the ice-atmosphere interactions are most sensitive. Our present thinking is that approximately ten thickness categories are needed if the ice thickness distribution is to be simulated in a manner consistent with the postulated viscous-plastic rheology of sea ice. The "order of magnitude" increase in the required computing time makes these simulations prohibitive on the computers of the generation of the CYBER 175.

Severe Storms, Tornados, and Downbursts (R. Wilhelmson)

The basic characteristic of storms which spawn tornados can now be simulated using CRAY-1 level computers [e.g. R. Wilhelmson (Univ. of Ill.) and others - calculations on NCAR CRAY]. The development, 3-dimensional structure, and movement of these storms can be modeled and compared with observed wind fields from Doppler radar. With enough supercomputer time, these studies can be extended to understand the detailed formation of tornados, hazardous downbursts, hail growth, and damaging surface winds associated with convective storms.

CHEMICAL ENGINEERING

Simulation of Wall Turbulence (T. Hanratty)

One of the exciting discoveries in the field of turbulence in recent years has been the discovery of coherent elongated flow structures close to a wall over which a turbulent fluid is flowing. It appears that these structures control the transfer of energy from the mean flow to the turbulence and therefore are a key to solving the turbulence problem. We have been trying to model these structures by solving the unaveraged time dependent Navier Stokes equations in a region close to a wall. By considering a limited region we do not have to use any closure models; however, we then have to specify the flow external to the wall region. Considerable success has been experienced in using a simple outer flow which is periodic in both time and space. We have expanded this work to include a flow field that is random in time. We now want to use an outer boundary condition which is random in space as well as time. A supercomputer at the U of I would make such a computation possible. One important aspect of this work is that it gives a physical insight as to how wall turbulence is produced. However, an equally exciting prospect is that it offers the opportunity of examining methods to control wall turbulence.

Chemical Process Flowsheeting and Optimization (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 the matrices arising in PDE problems to be so 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.

ELECTRICAL ENGINEERING

Circuit Simulation and Design Evaluation (S. Davidson)

I heartily support this effort to restore campus computing facilities to an adequate level in line with other eminent universities and research institutions. Such a plan would of necessity require a complete revision of how campus computing funds are allocated as well as new money. It involves new facilities and new easy access methods for obtaining computer time (e.g. on-going accounts for each student and each faculty member rather than a specific "course" accounts and semester-by-semester red tape and research accounts with a long lead time to set up).

Within our research group, our VAX and HP3000 computers 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. Continued operating budget for these systems is a constant problem even at present inadequate levels, e.g. for rapid maintenance. Computation intensive tasks such as circuit simulation and design verification and evaluation are extremely limited due to the low speed of these small computers. A CRAY system networked to our systems would provide this capability and would allow designs to be well evaluated prior to fabrication, thereby avoiding costly redesign cycles with can cripple our research effort. In coursework, such evaluation would give students invaluable feedback on their design errors. Supported local instructional and research facilities networked to a sophisticated number cruncher, like the CRAY X-MP, would be an ideal solution. The alternative is a continued deterioration of computing capability and hence of this university as a research and educational institution.

Simulation of 3-D Submicron Semiconductor Devices (K. Hess)

Our interest in three-dimensional modeling and graphical representation of submicron semiconductor structures by Monte Carlo techniques and self-consistent finite difference methods necessitates extensive and extremely fast computing facilities.

Inverse Problems (W.K. Jenkins)

We are involved with 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 in the design and performance evaluation of digital communications systems. For even moderately complex system models it may be possible to obtain only suboptimal de-

sign 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.

MECHANICAL AND INDUSTRIAL ENGINEERING

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 (10^{-6} seconds) 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.

THEORETICAL AND APPLIED MECHANICS

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 problem, 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.

Micromechanics of Ductile Rupture (R. McMeeking)

Fracture of ductile metals at ambient or high temperatures can occur by the nucleation, growth and coalescence of internal holes. These holes nucleate at inclusions in the material and the deformation of the holes is controlled by the mechanisms of plastic flow. My research is concerned with modelling the processes of rupture by analytic means. However, the governing equations are nonlinear and the geometries are complicated, especially when many

holes or a crack are present. It is necessary to solve the problems on a grid of finite regions whose behavior is calculated on the computer (finite element method). Currently because of memory and speed limitations, I am restricted to 2-dimensional problems with a limited number of cylindrical holes in very simple arrangements. Yet, the important problems concern the 3-dimensional interaction of ellipsoidal holes with each other and with other flaws such as major cracks. On a supercomputer, the extra storage would permit the solution of more realistic problems in more detail. This would include the interaction of holes with nearest neighbors, coalescence of holes with major cracks to cause crack propagation and the influence on hole deformation of individual anisotropic grains around a particular cavity. None of these problems is being tackled anywhere to my knowledge, yet they represent important phenomena in ductile rupture. A knowledge of the solutions would deepen our understanding of fracture and perhaps help us to improve the behavior of alloys. A supercomputer at UI would permit me to tackle these calculations.

CIVIL ENGINEERING

Synthesis and Optimization of Structural Systems (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 voluminous 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 and being 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 for investigation.

AERONAUTICAL AND ASTRONAUTICAL ENGINEERING

Rarefied Gas Dynamics (S. M. Yen)

We have developed the first and only accurate Monte Carlo method to solve directly the nonlinear Boltzmann equation for non-equilibrium gas flow problems. This method involves two explicit steps: to evaluate the Boltzmann collision integrals using a Monte Carlo method and to integrate the Boltzmann equation using a finite difference method. The Monte Carlo calculations required in the first step are time consuming, since a large sample is needed to accurately evaluate the collision integrals in the velocity space at each physical point in the flow field. So far we have successfully obtained accurate solutions of several one-dimensional flow problems. The solutions are significant in studying not only the detailed and often unforseen non-equilibrium gas behavior but also the validity of approximate methods useful for applications to engineering problems. We are now planning to apply our method to multi-dimensional problems which require many more nodes in the computational mesh. A supercomputer such as the CRAY X-MP, which has a large central memory as well as a buffer memory with high transfer rates, would be essential in the present phase of our study.

Computational Fluid Dynamics (S. M. Yen)

Our current interest in computational fluid dynamics is in solving a wide range of problems characterized by complexities in flow conditions, boundary conditions and flow geometries. Specifically, we have been studying numerical methods to solve nonlinear free surface wave problems in naval hydrodynamics, complex aerodynamic problems, viscous blast wave problems, and hypersonic flow problems. Our research has been handicapped by the lack of a large scale computer on campus. Frequently, we need such a computer to run some of the computer programs developed by others on related problems. The availability of a supercomputer such as the CRAY X-MP will enable us to make calculations for three-dimensional problems.

ANATOMICAL SCIENCES

Biomechanics of Cell Sheets (E. 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.

GENETICS AND DEVELOPMENT

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 the computer. The model is a great step foward 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.

Image Sequence Analysis of Living Cells (R.P. Futrelle)

On the experimental side we currently do image sequence analysis on a small scale. Further down the road, as we develop production quality software, we would like to analyze living cell behavior sequences of 100,000 frames containing a 1 Mbyte/frame. It may be that a supercomputer would play an important role here too, but it is a bit early to tell.

PHYSIOLOGY AND BIOPHYSICS

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 im-

portant 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.

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 numbers 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.