HIGH-PERFORMANCE COMPUTING AT THE MINNESOTA SUPERCOMPUTER INSTITUTE

Chaired by Lynne K. Edwards, *University of Minnesota*

Scientific computation: An interdisciplinary approach at Minnesota

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This paper summarizes the welcoming talk at the Symposium on High-Performance Computer Applications in the Behavioral Sciences. It provides a brief overview of selected activities in scientific computation at the University of Minnesota Supercomputer Institute. These activities include international symposia and a graduate degree program.

The Supercomputer Institute is an interdisciplinary research program spanning all colleges of the University of Minnesota. It supports and assists supercomputing research, which is taken in a broad sense to include a variety of activities from many disciplines. Supercomputer Institute research involves the use of high-performance computing environments to address problems in the physical, biological, and social sciences and in engineering that could not otherwise be attempted; such efforts often result in enhanced insight and understanding in the fields of application. Additional activities are aimed at the design or evaluation of high-performance computing hardware, operating systems, networking, and general-purpose algorithms and software. Resources are available to researchers at the University of Minnesota and other post-secondary educational institutions in the State of Minnesota, as well as their collaborators. The Institute also organizes and hosts symposia, workshops, and seminars and coordinates other activities to promote supercomputer research, increase university-industry collaboration, and promote technology transfer. The Institute offices are located primarily in the Minnesota Supercomputer Center in the Minnesota Technology Corridor in Minneapolis.

The University of Minnesota pioneered in the operation of supercomputers in an academic environment. We were the first U.S. university to acquire a supercomputer, a Cray-1B, installed in 1981. Since that time, we have provided our researchers with access to a sequence of high-performance architectures produced by Cray Research,

Control Data Corporation, ETA, IBM, Thinking Machines, and Silicon Graphics. The Institute has also provided extensive support facilities, including an advanced communications network and workstations and graphics systems produced by Silicon Graphics, SUN, Apple, NeXT, and IBM. Institute researchers with a broad range of interests are using state-of-the-art facilities to produce a large amount of exciting research in many fields.

The scope of supercomputing activity is illustrated by the breadth of the current Institute research program. This year we have 189 faculty principal investigators from 41 departments and 11 colleges. Examples of current and recent projects that may be of interest to the current audience are our research programs from the Departments of Educational Psychology, Environmental and Occupational Health, Industrial Relations, Operations and Management Sciences, and Pharmacology, in the Carlson School of Management, the College of Education, the College of Liberal Arts, the Medical School, and the School of Public Health. These research projects include studies of Monte Carlo methods applied to educational statistics, estimation of discrete stochastic dynamic programming models of economic behavior using Monte Carlo integration, sequential multivariate statistical methods for simulation output analysis with guaranteed precision, approximation-assisted point estimation, robust parameter selection for compartmental models of neurons using evolutionary algorithms, protein structure estimation using homology and neural networks, performance strategies for selecting models when analyzing epidemiological data, and numerical studies of airborne particle transport in near bluff flow obstacles.

An activity that may be of interest is the Graduate Program in Scientific Computation. This program encom-

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passes course work and research on the fundamental principles that enable the use of intensive computation in research in the physical and social sciences and engineering. There is a special emphasis on research issues, state-of-the-art methods, and the application of these methods to outstanding problems in science, engineering, and other fields that use numerical analysis, symbolic and logic analysis, high-performance computing tools, parallel algorithms, supercomputing and heterogeneous networks, and visualization. The Scientific Computation program offers MS and PhD degrees.

Scientific computation is now emerging as an important field of its own in academia and industry. In recent years, it has become more and more clear that to solve a given scientific problem often requires knowledge that straddles several disciplines, and, in response to this observation, our scientific computation degree program provides a new combination of studies for solving today's scientific computational problems. This program joins field-specific work in formulating real problems based on the physical system or the traditional discipline with state-of-the-art techniques for numerical analysis and computation. Students are encouraged to form a strong association with one or more of the home departments of participating faculty, who are drawn from the Departments of Aerospace Engineering and Mechanics, Agricultural Engineering, Astronomy, Biochemistry, Chemical Engineering and Materials Science, Chemistry, Civil Engineering, Computer Science, Educational Psychology, Electrical Engineering, English as a Second Language, Geology and Geophysics, Mathematics, Mechanical Engineering, Medicinal Chemistry, Operations and Management Science, Psychology, Sociology, and Statistics.

It may also be of interest to see how the present symposium fits into the Supercomputer Institute's ongoing efforts to promote interdisciplinary communication and to advance the state of the art in scientific computation through national and international symposia and workshops. We have sponsored symposia and workshops on the following topics:

- finite element methods in large-scale computational fluid dynamics
- neural networks for physicists
- computational molecular dynamics
- domain-based parallelism and problem decomposition
- methods in computational science and engineering
- parallel finite element computations
- modeling, mesh generation, and adaptive numerical methods for partial differential equations
- finite element methods and other developments in large-scale computational fluid dynamics
- visualization and statistical analysis in hard turbulence
- parallel computing
- iterative methods for sparse and structured problems
- computational approaches in molecular biology and biophysics

- large-scale computations applied to many-body systems
- simulation of semiconductor devices
- chaotic processes in the geological sciences
- nonlinear phenomena in atmospheric and oceanic sciences
- visualization and graphics
- supercomputer protein chemistry
- potential energy surfaces and chemical dynamics
- modeling for conservation laws in continuum mechanics
- practical iterative methods for large-scale computations
- supercomputing and large-scale optimization
- supercomputing in biology: proteins, nucleic acids, and water
- supercomputer research in chemistry and chemical engineering

To which we can now add:

- supercomputer applications in the behavioral sciences

In addition, we currently have international symposia or workshops planned on:

- new methods in electronic structure calculations
- mathematical and computational issues in drug design
- evolutionary algorithms (including genetic algorithms)
- modeling in biochemical engineering
- parallel scientific computation

Most of these symposia and workshops have involved interdisciplinary groups and mixtures of researchers from academic, industrial, and government sites. In my opinion, the cross-fertilization that has occurred has been significant, and we plan to try to continue to encourage this kind of activity in the future. We invite all interested researchers to suggest topics for future symposia and workshops that would be of interest.

The first talk given at the present symposium was very remarkable to me in reinforcing how profitable it can be for computational scientists from widely disparate backgrounds to share their experiences. The speaker, Richard Shiffrin, described a series of steps in the development of a computational model in the behavioral sciences, and at every step of the way I found a shock of recognition as the very same problems had occurred in our own recent work on developing models for computing free energies of solvation of organic molecules in aqueous solution. Not only are the problems the same, but Shiffrin's "behind the scenes" commentary on how he attacked the problems showed some intriguing similarities to our own model building. I found especially familiar the description of how they "operated under the speed constraints in a highly interactive and intuitive manner, obtaining predictions for relatively few parameter sets, thinking about the results, choosing a few additional parameter values for exploration, and so forth," with the goal of training their own understanding of the model's structure and perhaps even leading to a decision to abandon their current model in favor of an alternative. This kind of process occurs in our chemical work, too. Interestingly, in the next

step, Shiffrin's program got "stuck" in local minima, and he turned to genetic algorithms. This too occurred in our own work. The analogy continued throughout his talk.

Shiffrin's talk left me more convinced than ever of the importance of sharing experiences across traditional boundaries. It was my impression from speaking to participants that the other talks at the symposium were also

very successful in stimulating the audience in various ways. I therefore close with special thanks to the organizers, Lynne K. Edwards of the University of Minnesota, Stephen W. Link of the Federation of Behavioral, Cognitive and Psychological Sciences, and Cynthia Null of NASA Ames Research Center, for providing this forum for the interchange of new ideas in computational science.