Third US-Japan Symposium on Finite Element Methods in Large-Scale Computational Fluid Dynamics

The Third US-Japan Symposium on Finite Element Methods in Large-Scale Computational Fluid Dynamics was held at the Army High Performance Computing Research Center (AHPCRC) from Sunday March 31 through Wednesday April 3, 1996. The Symposium was sponsored by the Department of Aerospace Engineering and Mechanics, AHPCRC and the Supercomputer Institute at the University of Minnesota. The organizing team consisted of Tayfun Tezduyar, Department of Aerospace Engineering and Mechanics and AHPCRC, Mutsuto Kawahara, Chuo University, and Thomas Hughes, Stanford University. The same team also organized the two earlier symposia in this series, which were held in October 1992 at the University of Minnesota and in March 1994 at Chuo University in Tokyo.

The symposium began on Sunday evening with registration and a welcoming reception held at the Marquette Hotel in downtown Minneapolis. Approximately ninety researchers from the United States, Japan, and Europe attended the symposium.

The symposium kicked off the following morning with welcoming and introductory remarks by Ettore Infante, Senior Vice President for Academic Affairs, Tezduyar, and Donald Truhlar, Department of Chemistry and Supercomputer Institute. The first session was chaired by Hughes, and presenters included Kawahara, Akira Maruoka of Chuo University, and Philip Gresho of Lawrence Livermore National Laboratory. The presentations were on the following subjects: "Future Trends in Finite Element Analysis" (Kawahara); "An Optimal Control Problem in the Navier Stokes Equation" (Kawahara and Maruoka); and "Projection Two Goes Turbulent-and Fully Implicit" (Gresho).

Gresho was chairperson of the second morning session. The first talk was given by Tezduyar and Vinay Kalro, on "3-D Flow Simulations on Parallel Platforms," followed by a talk given by Kazuo Kashiyama (Chuo University) on a "Massively Parallel Finite Element Method for Storm Surge." The last presentation of the morning was on a "Parallel Overlapping Scheme for Viscous Incompressible Flows," given by Masayuki Kaiho of Hitachi.

The first afternoon session was chaired by Kashiyama and began with a talk given by Andrew Johnson of the AHPCRC on "Parallel Computation of Incompressible Flows with Complex Geometries." Following Johnson was John Shadid of Sandia National Laboratories. Shadid presented his work on "Fully-Coupled Iterative Solution of Chemically Reacting Flows on Massively Parallel Supercomputers."
The fourth and final session of the day was a panel discussion on the "Role of Flow Simulation," chaired by Robert Whalin of the Corps of Engineers Waterways Experiment Station (CEWES). The other panelists included H. Ted Davis, Dean of the Institute of Technology at the University of Minnesota, Kawahara, and William Mermagen of the Army Research Laboratory (ARL).

"US-Japan Symposium article" continued

Symposium on Supercomputer Applications in the Behavioral Sciences held May 10-12, 1996

This symposium was a follow-up to the 1985 National Science Foundation conference Advanced Computing for Psychology, which examined the increasing importance of high-performance computers, including workstation clusters, in the behavioral sciences. At the current conference, held Friday, May 10 through Sunday, May 12, 1996 at the Supercomputer Institute, representative topics included computer-intensive simulation methods, virtual reality, human factor, neural networks, brain magnetic resonance imaging, information processing, large data handling, perception and human vision, and graphic visualization in the behavioral sciences. This symposium was sponsored by the University of Minnesota Supercomputer Institute, the College of Education and Human Development, and the Federation of Behavioral, Cognitive, and Psychological Sciences. The organizing committee consisted of Lynne Edwards, Department of Educational Psychology and the Supercomputer Institute; Stephen Link, Federation of Behavioral, Cognitive, and Psychological Sciences; and Cynthia Null, NASA Ames Research Center.

In addition to talks, presentations, and discussions, the symposium included tours of high-performance computing facilities at the University of Minnesota. These included the IBM Workstation Cluster, the Laboratory for Computational Science and Engineering, and the supercomputing facilities at the Minnesota Supercomputer Center Inc.

The presentations began on Saturday morning with welcoming speeches by Donald Truhlar, Director of the Supercomputer Institute and Department of Chemistry, followed by Cynthia Null, NASA Ames Research Center, who was also a co-organizer for the 1985 Conference on Advanced Computing for Psychology, and Stephen Link, Federation of Behavioral, Cognitive and Psychological Sciences, who participated in the 1985 NSF conference. Richard Shiffrin and Peter Nobel, both of the Department of Psychology at Indiana University, discussed methods for building mathematical models of human memory. They spoke about the function of high-performance computing in models and testing of those models. These talks illustrated the emergence of scientific computation as a cross-disciplinary field in its own right since many of the problems and experiences presented were similar to those encountered in model-building endeavors in other disciplines.

Later that morning, Richard Golden of the School of Human Development at the University of Texas at Dallas, described a Markov random field probabilistic model in which subjects recall events in a text from memory.

James Cutting of the Department of Psychology at Cornell University used various paintings to show that the human visual system exhibits tolerance for some deviations from a Euclidean representation of space and an intolerance for others. In the pictures, perception cues were provided by occlusion, height in the visual field, relative sizes and densities, binocular disparities, motion perspectives, and the like.
Daniel Kersten of the Psychology Department at the University of Minnesota, gave a presentation of 3-D animation tools which produced realistic movies with strong perceptual cues. The goal of Kersten's work is to increase understanding of the human visual system by observing the cues and responses by viewers. Kersten applied Bayesian analysis to understand the identity of objects and their spatial relationships by cues such as cast shadows.

In the afternoon on Saturday, Mary Kaiser of the NASA Ames Research Center, Moffett Field, California, discussed how the visualization of a particular data set-the Digital Terrain Model of Mars, which was derived from the Viking Orbiter imagery-can be optimized using our knowledge of human perception.

Jeffrey Mulligan, also from the NASA Ames Research Center, demonstrated the use of a video camera to track human eye movements. He noted that a major bottleneck is the real-time digitization and storage of large video imagery, but that recent developments in video compression hardware have made it less expensive and easier to manage these tasks. Images from the retina and the pupil can be analyzed with a basic image processing tools such as filtering, correlation, and thresholding-all of which are well-suited for implementation on vectorizing supercomputers.

Sam Williamson, Department of Physics and Center for Neural Science, New York University, presented magnetic source images (MRI) of human brain functions. Williamson is using large arrays of superconducting magnetic field sensors to map the topography of the magnetic field pattern across the human scalp.

James Anderson, Department of Cognitive and Linguistic Sciences, Brown University, focused on neural network models. He noted that although there are some good computational theories for the behavior of single neurons and that some large-scale aspects of their behavior seem lawful, there is no theory for connecting the behavior of a single neuron to the behavior of 10^11 neurons at work in the human brain. Anderson commented on the fact that as currently formulated, neural networks seem to lack essential mechanisms necessary for flexible control of the computation and neglect structure at intermediate scales of organization.

The talks began on Sunday with a presentation by Albert F. Anderson, Population Studies Center, University of Michigan, Ann Arbor. Anderson provided a real-time demonstration of a software interface for accessing and analyzing the census data via SP2 and workstation clusters. He also presented a fast data mining system for a broad spectrum of users.

Later Sunday morning, James Ramsey, Department of Psychology, McGill University, discussed a suite of techniques that promise to advance the power and scope of function estimation, while presenting interesting computational challenges.

The symposium was concluded by Patrick Suppes of Stanford University. Suppes compared the computational loads involved in the human vision system to those of analyzing turbulence in physics. He also pointed out that while human vision in naturally rich contexts is now simulated and analyzed, the work on human memory is still limited to an artificial laboratory context. There is a great need for the research on memory to play "catch-up"to research on human vision. Another area awaiting further research is that of brain magnetic resonance imaging (MRI), which involves the measurement and visualization of electromagnetic activities in the brain. He pointed out that there is not yet a meaningful correlation made between the underlying psychological processes and specific electromagnetic activities in the brain.

The symposium was opened with an overview of high-performance computer architectures presented by representatives from Cray Research Inc., Silicon Graphics Inc., and IBM. The sessions were chaired by Stephen Link, Federation of Behavioral, Cognitive, and Psychological Sciences; Al Yonas, Institute
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of Child Development, University of Minnesota; Cynthia Null, NASA Ames Research Center; Jay Samuels, Department of Educational Psychology, University of Minnesota; Mark Davison, Department of Educational Psychology, University of Minnesota; and Lynne Edwards Department of Educational Psychology, University of Minnesota and the Supercomputer Institute. This conference was successful in fostering interactions among speakers and the attendees on high-performance computing in the behavioral sciences. An active discussion followed each presentation. The symposium ended with closing remarks by Lynne Edwards, chair of the organizing committee, and the announcement of the symposium proceedings in early 1997.

Upcoming Symposium

International Conference on Parallel Computing, October 3-4, 1996

The Supercomputer Institute and IBM Corporation are sponsoring the International Conference on Parallel Computing from October 3-4, 1996. The conference, formerly scheduled to take place in San Jose, California in August, has been moved to Minneapolis.

The conference will bring together scientists and post-graduate students to discuss distributed parallel applications in computational sciences and to foster cross-disciplinary interactions in the general area of high-performance computing. There will be a mix of talks dealing with novel programming and algorithmic aspects as well as state-of-the-art technical advances. Invited speakers will be from around the world and are currently being contacted. This will be a concentrated forum to discuss progress on enhancing the number of applications that run in parallel.

For further information, please refer to the ICPC World Wide Web announcement.

Summer Undergraduate Interns Arrive and Begin Work on Research Projects

The Supercomputer Institute welcomed its summer interns to the program on Wednesday, June 19, 1996 with an orientation session and social hour. The interns come from diverse academic backgrounds but share an interest in science and computational approaches to solving problems in engineering, physics, chemistry, mathematics, and biochemistry. They come from colleges and universities across the nation, including Brown University, University of California-Berkeley, Cooper Union for the Advancement of Science and Art (New York City), Harvard University, Princeton University, Rochester Institute of Technology, University of Rochester, University of Minnesota, and Augsburg College.

There were 155 applications for this summer's program and appointments were made for 14 applicants. Of those, eight are from outside of Minnesota, one is from a Minnesota college other than the University of Minnesota, and five are from the University of Minnesota. The National Science Foundation provides support.

Description and History of Program

The Supercomputer Institute's Undergraduate Internship Program in Scientific Computing and Graphics
was started in 1990. It provides special opportunities for undergraduate participation in the Supercomputer Institute's state-of-the-art interdisciplinary research programs. During the summer, interns work 40 hours per week, immersing themselves in high-performance computing research as it relates to their field of interest. The goal of this program is to attract talented undergraduates to science and engineering careers, to encourage undergraduates to attend graduate school in science and engineering, and to enhance undergraduate education. All interns work closely under the direction of their faculty project supervisor and the supervisor's research group.

Project Descriptions

Following is an introduction to our summer interns, including brief descriptions of the projects they are working on.

Linda Addis, a junior at the University of Minnesota majoring in Chemical Engineering is working in Professor Chris Cramer's chemistry research group on a project titled "Stereochemical Effects on Equilibria and Reaction Kinetics" Also working in chemistry is Molli Noland, a junior at Rochester Institute of Technology, Rochester, New York. Noland is majoring in Computational Mathematics and is a member of Professor Donald Truhlar's research group working on a project involving correlated capped subsystem methods for direct dynamics calculations on large systems.

Marwane Berrada, a Mechanical Engineering junior at the University of Minnesota is doing research with Professor Joachim Heberlein on "Thermophysical Properties of Mixtures."

Kevin Chou is an Electrical Engineering junior at Cooper Union for the Advancement of Science and Art in New York City. He is working with Professor Ahmed Sameh in the Department of Computer Science. Their work involves developing and optimizing algorithms for solving the symmetric indefinite linear systems that arise from constrained optimization problems.

Steven Clayton, a junior at the University of Minnesota majoring in Physics, is working with Professor J. Woods Halley on a project entitled "Simulations of Chemical and Cryogenic Systems." We note that Clayton successfully concluded a different project in Spring Quarter in which he developed a keyword-controlled input protocol for direct dynamics calculations with the POLYRATE direct dynamics code under the direction of Professor Donald Truhlar of the Chemistry Department and University of Minnesota Supercomputer Institute Research Scholar Laura Coitiño.

G. Stuart Mendenhall is a Harvard junior majoring in Chemistry and Physics. His faculty supervisor for the summer is Professor Professor Leonard Banaszak, Department of Biochemistry. Their project is titled "Computer-Assisted Interpretation of X-Ray Diffraction Data in Protein Crystallography."

Elizaveta Pachepsky, a junior at the University of Rochester majoring in Mathematics is working on a fractals project with Professor David Yuen's Geology and Geophysics research group.

Julie Patterson comes to Minnesota from Princeton University where she is a junior majoring in Chemical Engineering. She is working with Professor David Ferguson in the Department of Medicinal Chemistry on a project which involves the simulation of HIV proteins. There are two interns working in the field of Aerospace Engineering and Mechanics. They are Larye Pohlman, an Augsburg College junior majoring in Physics, and Natasha Shekdar, a senior at Brown University majoring in Civil Engineering. Pohlman is working with Professor Graham Candler on a project titled "Simulation of Chemically Reacting Flows." Shekdar is working in Professor Tayfun Tezduyar's research group. Their work involves parallel finite element simulations of fluid flow applications.

Agustinus Sutandi is a junior at the University of Minnesota majoring in Chemical and Electrical Engineering. Sutandi is working with Professor Jeffrey Derby's Chemical Engineering research group. Their project involves developing visualization software for finite element models of materials.
processing systems

**Vincent Voelz** is a senior at the University of Minnesota majoring in Math and Physics. He is working with Professor David Thomas, Biochemistry (Medical School). Their project involves supercomputer simulations of muscle molecular biophysics to augment their laboratory work on force generation and movement in muscle.

**Danny Yang** is a senior from Harvard working with Professor Bill Gleason on a project titled "Homology Modeling Studies of Oncogenic Heparin-Binding Proteins Based on Crystal Structures of Fibroblast Growth Factors."

For more information on the Supercomputer Institute's Summer Undergraduate Internship Program, please contact the Undergraduate Internship Coordinator.

Coordinator
Undergraduate Internship Program
Supercomputer Institute
1200 Washington Ave. South
Minneapolis, MN 55415
Tel: (612) 626-7620
E-mail: uip@msi.umn.edu

You may also reference our Internship Program World Wide Web page.

### Seminar Synopses

- Christopher R. Johnson, Computer Science Department, University of Utah, Salt Lake City, Utah
  Large-Scale Modeling, Computation, and Visualization in Medicine

- David H. Bailey, NASA Ames Research Center, Moffett Field, California
  Using Supercomputers to Discover New Mathematical Identities

- Peter M. Goorjian, NASA Ames Research Center, Moffett Field, California
  Computational Modeling In Nonlinear Optics of Ultrafast Pulse Propagation

- Evan Mitsoulis, Department of Chemical Engineering, University of Ottawa, Ottawa, Ontario, Canada
  Recent Advances in the Numerical Simulation of Viscoelastic Flows with Integral Constitutive Equations

- Stanley Osher, Mathematics Department University of California, Los Angeles, California
  The Scope of the Level Set Method for Computational Fluid Dynamics

- Irwin Kuntz, Pharmaceutical Chemistry Department, University of California, San Francisco, California
  Structure-Based Molecular Design

- Olaf O. Storaasli, Langley Research Center, Hampton, Virginia
  High-Performance Equation Solvers for Aerospace Analysis and Design (Structures and Electromagnetics)

- Kisa Matsushima, Department of Supercomputer Systems, FUJITSU Ltd., Tokyo, Japan
  High Performance Flow Simulation and Its Incorporation into Design Problems

- Steve Reinhardt, Cray Research, Eagan, Minnesota
Overview of the Cray T3E

Large-Scale Modeling, Computation, and Visualization in Medicine
Christopher R. Johnson
Computer Science Department
University of Utah
Salt Lake City, Utah

Computer modeling and simulation of problems in medicine often require a researcher to apply diverse skills in confronting the challenges associated with large data sets, three-dimensional complex geometries, large-scale computing, and numerical analysis. The speaker presented an overview of these distinct, but interrelated aspects of large-scale problems in computational medicine, concentrating on bioelectric field applications in cardiology and neuroscience.

Using Supercomputers to Discover New Mathematical Identities
David H. Bailey
NASA Ames Research Center
Moffett Field, California

Oddly, the field of pure mathematics has been one of the last scientific disciplines to embrace the computer as an essential research tool. This is changing with the emergence of powerful symbolic math packages and a new generation of computer-literate mathematicians.

This presentation described the discovery of new mathematical identities by means of numerical computations on workstations and parallel supercomputers.

Computational Modeling In Nonlinear Optics of Ultrafast Pulse Propagation
Peter M. Goorjian
NASA Ames Research Center
Moffett Field, California

Goorjian described algorithm development and computed results in computational nonlinear optics. The computer simulations he discussed are made by solving the full-vector, nonlinear Maxwell equations without any approximations. For the light bullet calculations, the Maxwell equations are coupled to nonlinear ordinary differential equations that model linear dispersion as well as nonlinear effects. For the calculations modeling semiconductors, the Maxwell equations are coupled to the semiconductor Bloch equations, without any approximations.

Recent Advances in the Numerical Simulation of Viscoelastic Flows with Integral Constitutive Equations
Evan Mitsoulis
Department of Chemical Engineering
In recent years progress has been achieved in the viscoelastic simulation of polymeric liquids by using integral constitutive equations. This is particularly true for the modelling of polymer solutions and melts with a spectrum of relaxation times. Novel numerical techniques based on the finite element method (FEM) have been developed to handle the necessary particle tracking in the general case of flows with open and closed streamlines. Test cases for commercial polyethylene melts have shown the adequacy of integral models to capture memory phenomena and strong viscoelastic behaviour, not seeing with simple models of the Upper-Convected Maxwell or Oldroyd-B types.

Considerable success in modelling viscoelastic flows has been achieved with a particular type of integral constitutive equation, proposed by Papanastasiou, Scriven, and Macosko, and referred to as the PSM model. This equation has been used to predict several well-known viscoelastic phenomena for polymer melts, such as extrudate swell, difference in behaviour between different polymer melts in flows through contractions, etc. It has also been used in the modeling of several polymer processes, such as fiber spinning, film casting, film blowing, etc.

This talk made an effort to explain from the numerical point of view past and current achievements in viscoelastic simulations of polymer fluid flows, mainly for two-dimensional, steady-state cases. Mitsoulis also discussed future developments and challenges in the field of computational non-Newtonian fluid dynamics.

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The Scope of the Level Set Method for Computational Fluid Dynamics
Stanley Osher
Mathematics Department
University of California
Los Angeles, California

In 1987, this speaker, together with J.A. Sethian devised a new numerical procedure for capturing fronts and applied it to curves and surfaces whose speeds depend on local curvature. The method has been applied to a very general class of problems in computational fluid dynamics.

The technique handles topological merging and breaking, works in any number of space dimensions, does not require that the moving surface be written as a function, captures sharp gradients and cusps in the front, and is relatively easy to program. Many applications and extensions have recently been found and were discussed in the talk.

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Structure-Based Molecular Design
Irwin Kuntz
Pharmaceutical Chemistry Department
University of California
San Francisco, California

Macromolecular structures contain detailed information that can be used to guide the design of low molecular weight compounds that bind specifically to “active sites” and other surface features.
Macromolecule-macromolecule interactions can also be studied. The basic computational tools are rigid and flexible docking programs that scan large databases of commercially available compounds or virtual libraries of compounds that are synthetically accessible. Professor Kuntz described the computational challenges in developing successful docking strategies with special emphasis on the new issues posed by the use of combinatorial libraries.

High-Performance Equation Solvers for Aerospace Analysis and Design (Structures and Electromagnetics)
Olaf O. Storaasli
Langley Research Center
Hampton, Virginia
This speaker described the development and performance of a new family of NASA-developed equation solvers used for large-scale (e.g., 551,705 equations) structural analysis. To minimize computer time and memory, the solvers are divided by application and matrix characteristics (sparse/dense, real/complex, symmetric/nonsymmetric, size: in-core/out of core) and exploit the hardware features of current and future computers.

In this talk, the equation solvers, which are written in FORTRAN and are therefore easily transportable, were shown to be faster than specialized computer library routines utilizing assembly code.

High Performance Flow Simulation and Its Incorporation into Design Problems
Kisa Matsushima
Department of Supercomputer Systems
FUJITSU Ltd.
Tokyo, Japan
This speaker presented two topics involving computational fluid dynamics applications. One concerned the flow field prediction of a future flight vehicle by vector parallel computation; the other was a direct design method in which a flow simulation solver and an inverse design solver are incorporated.

The first topic dealt with compressible viscous flows past a space plane, one of Japan’s SST/HST candidates, simulated on a Japanese vector parallel supercomputer. The second topic dealt with the aerodynamic design of wing sections whose geometry realizes a specified surface pressure distribution with a given flow condition. In addition, several examples of aerodynamic design of wing systems were discussed.

Overview of the Cray T3E
Steve Reinhardt
Cray Research
Eagan, Minnesota
The Minnesota Supercomputer Center Inc. is scheduled to install a Cray T3E Massively Parallel Processing supercomputer in the Spring of 1997. Steve Reinhardt, the T3E Project Director at Cray Research Inc. was the feature presenter at a recent gathering of the Minnesota Supercomputer Institute.
and Minnesota Supercomputer Center Inc. He presented an historical account of Cray Research's Massively Parallel Processing project and provided some of rationale behind its design decisions for the T3D and subsequent T3E project.

He stated that the T3D design emphasized high bandwidth between processors as well as small latencies for interprocessor communication. These design parameters were also an important part of the T3E design, but there was a much larger emphasis on single processor performance. He overviewed Cray's hardware and software strategy for accomplishing increase single processor performance. He also emphasized the specific application areas where the T3E is expected to perform well.