Spring 2001

The Resource

U.S. ARMY ENGINEER RESEARCH AND DEVELOPMENT CENTER NEWSLETTER

ERDC MSRC

Major Shared Resource Center

From the Director's chair

The cover of this newsletter highlights new leadership and new technology. The Department of Defense (DoD) is in good company with the Bush/Cheney team; General Flowers, the new Chief, Corps of Engineers (COE), has a vibrant new vision for the COE and promotes a "Just Do It" philosophy; and the new Director of the Engineer Research and Development Center (ERDC), Dr. James Houston, has a strong commitment to high-performance computing (HPC). Cray Henry has been the Director, High Performance Computing Modernization Program (HPCMP), for about a year and a half. More recent additions and new assignments to the High Performance Computing Modernization Office (HPCMO) are Dr. Larry Davis as the Deputy Director, Dr. Frank Mello, Chief Scientist, and Dr. Leslie Perkins, Programming Environment and Training (PET) and Common High Performance Computing Software Support Initiative (CHSSI) Lead. This new team brings diverse talent with management experience, historical HPCMP knowledge, technical expertise, and computational expertise to the HPCMP leadership roles. With this strong cadre of new faces in high places, we are in a good position to embrace future challenges.

On the technology side, I want to use the rest of this space to highlight a technology that has been in the minds of HPC people for over two decades—grid computing. It all started with the interconnection of computers with "networks." In the early days, DECnet was a leader. Anybody remember LAT? Although DECnet is still around, transport control protocol/Internet protocol (TCP/IP) "stacks" (I always think of pancakes when I hear this) eventually provided a standards-based foundation for inter-networking. Yes, some distractions occurred along the way; but when the going got tough, TCP/IP always surfaced. The big thrust now is "grids." This is more commonly known as metacomputing, but the community quickly learned that metacomputing meant too many things to too many people. A technology that is manageable is grid computing. Initially, this was termed "computational grids," but I shy away from this, as it steps on the turf of the computational scientists who construct computational grids for numerical solutions. Hence, we move forward with "grid computing." What is it? We all know that most of our computers are physically connected together with networks. Grid computing is layers of functionality on top of the network that provide the end user the ability to couple resources together to address a problem or system of problems. Computers are the most common resources, but devices like a network-attached microscope or a measuring instrument can also contribute.

The HPCMP is in the early stages of building a computational grid. This requires a "melding" of the infrastructure that involves not only the hardware and software technologies but the policies, operating procedures, and people. The whole community must begin to think about grid computing and what their role is. Configuration control, security, user services, applications, user interfaces, and accounting to mention just a few are all impacted. Most importantly, the user will be impacted. The computing environment will become more complex and will offer a capability far above what is possible with today's infrastructure. Grid computing will be an evolutionary capability. In the future, grids will be interconnected with other grids. You will someday be able to "borrow" a telescope from the National Aeronautics and Space Administration (NASA) for a few hours. The possibilities are endless.

We have great new leadership and great new technologies. Look for the two working together to change the way we do HPC.

Bradley M. Comes
Director, ERDC MSRC

About the Cover:
New Leadership. (Front row, left to right) United States President George W. Bush; Dr. Leslie Perkins, PET and CHSSI Lead, HPCMP; (back row, left to right) General Robert B. Flowers, Commanding General, U.S. Army Corps of Engineers; Dr. James R. Houston, Director, ERDC; Cray Henry, Director, HPCMP; Dr. Frank Mello, Chief Scientist, HPCMP; and Dr. Larry Davis, Deputy Director, HPCMP (see article, page 6).
New Technology. (Left to right) Mass Storage Facilities, Origin 3800 Supercomputer, and SC2000 DoD HPCMP Booth (see articles, pages 8, 24-30).

Features

Departments

Rebecca Fahey Accepts Position as Director of User Services

Rebecca Fahey recently accepted the position of Director of User Services. In this position, she will oversee the Customer Assistance Center, Applications Analysts, and Database Group.

Rebecca brings a significant amount of technical expertise to the position. She transferred to the position from the Computational Migration Group at the ERDC Major Shared Resource Center (MSRC), where she assisted users in the development, migration, and optimization of parallel codes. Prior to this position, Ms. Fahey taught in the University of Kentucky system, where she was involved in several projects designed to integrate more technology into the classroom.

Rebecca's technical expertise will blend nicely with the activities of User Services. Rebecca's current goal is to develop the technical skills of the Customer Assistance Specialists to be more in tune with the needs of the user community through a new support model that puts much more emphasis on direct front-line support versus managing customer calls through a hierarchical tree of expertise.

Mark Green Joins the ERDC MSRC

Mark Green joined the ERDC MSRC in October 2000. Mark's focus is serving as the MSRC's POC for networking and mass storage systems.

Mark has worked at ERDC for 22 years. He began in 1979 as a student trainee and then, upon graduation, joined the professional staff in 1982. Prior to joining the MSRC team, he served as a research civil engineer in the Geodynamics and Explosion Effects Division of the ERDC Geotechnical and Structures Laboratory, where he conducted numerous investigations to characterize the response of geologic materials subjected to explosive loadings and to understand the effects of projectile penetration into geologic targets. He has authored and coauthored 20 technical reports and papers and is a registered professional engineer in the State of Mississippi. Mark graduated from Mississippi State University with B.S. and M.S. degrees in civil engineering and completed 1 year of advanced study in geotechnical engineering at the University of Colorado.

New Lead on Grid Computing Development and Systems Operation

Greg Rottman joined the ERDC MSRC as a civil engineer in June 2000. He has worked 4 years in engineering and has had 13 years of experience in information technology and 5 years in project management. Greg supports systems operations and serves as the lead on developing grid computing capabilities throughout the HPCMP.

After graduating from Texas Tech University with a B.S. degree in agricultural engineering, Greg worked as a hydraulic engineer for the U.S. Army Corps of Engineers in Fort Worth, Texas. In 1981, he accepted a position as a civil engineer in the Automated Data Processing Center (ADPC) in Fort Worth as a liaison between the ADPC and the Engineering Division. He went to work for Tektronix, Inc., Graphics Workstation Division, in 1984 as a systems analyst. After 7 years, Greg returned to Government service at the ERDC Information Technology Laboratory (ITL), where he worked in Customer Assistance and served as project engineer and project manager for the Electronic Information Exchange Project. He then worked for 5 years in the Programs and Project Management Division at the U.S. Army Engineer District, Vicksburg, before returning to the ERDC to work in the MSRC.

Deputy Program Manager Named

In August 2000, John Mauldin joined the Computer Sciences Corporation (CSC) and assumed the responsibilities of Deputy Program Manager for the MSRC integration contract. John brings a wealth of technical knowledge and experience to the program and will provide much insight.

John earned his B.S. degree in electrical engineering and M.S. degree in computer science from Mississippi State University. He began his career as an electrical engineer with RCA Missile and Surface Radar in Moorestown, New Jersey, where he developed automated testing software for production-environment, quality assurance testing of radar components. John later spent 11 years with Nichols Research Corporation in Huntsville, Alabama. There he progressed from a technical contributor into management. His previous experience includes working on the ERDC and Aeronautical Systems Center (ASC) HPC integration proposal team. Prior to coming to Vicksburg, he worked for Sword Microsystems in Huntsville, Alabama, as the Chief Operating Officer and Vice President for Technology and Development. There, he also served as Program Manager providing a Web-based on-line ordering system used in business-to-business transactions for a large printing company, which was successfully prototyped and delivered. Throughout his career, John has also gained experience in technical consulting in the areas of eBusiness strategies, business process analysis, and re-engineering.

While in the Huntsville area, John took an active role in the North Alabama Habitat for Humanity organization and served as the President of the Board of Directors for 6 years. During his tenure as President, over 25 houses were completed.

Outside of the office, John enjoys spending time with his wife, Karen, and their three daughters, Anna, Becca, and Ali.

Upcoming Events

Jackson State University High Performance Computing Summer Institute — June 4-15, 2001

SC2001 Conference — "Beyond Boundaries," November 10-16, 2001 Denver, Colorado, SC Goes Global

Users Group Conference 2001 — June 18-21, 2001, Beau Rivage Resort Biloxi, Mississippi

Current Trends in Computational Chemistry 2000

The 9th Conference on **Current Trends in Computational Chemistry** was held in Vicksburg, Mississippi, on November 3-4, 2000. This symposium was organized by the ERDC MSRC PET Program partner Jackson State University, one of the Historically Black Universities and Colleges/Minority Institutions (HBCU/MI). The conference covered all areas of computational chemistry as well as quantum chemistry. The local host of the conference was the ERDC headquarters at Waterways Experiment Station in Vicksburg.

Dr. Phu Luong, ERDC MSRC, presented a virtual reality visualization of a Persian Gulf simulation using the Princeton Ocean Model (POM) for the conference participants in the Collaboratorium located in ITL.

Collaboration/Communication Tutorial

Professor Geoffrey Fox, Florida State University, presents tutorial at the ERDC MSRC

As part of the ERDC MSRC PET Program, Professor Geoffrey Fox, Florida State University, presented a tutorial at the ERDC MSRC on March 1, 200l. The current, state of the art in collaboration and communication was presented. The tutorial included systems, tools, and standards for distributed meetings, training and education, wireless communication technology, and high-quality digital audio and video over the Internet. The Access Grid project was discussed along with the complex requirements for group-to-group interactions and the creation of a distributed virtual environment.

Lectures on Parallel Adaptive Algorithms and Software Frameworks for DoD Challenge Class Applications

Dr. Robert T. McLay, a research associate at the Texas Institute for Computational and Applied Mathematics, University of Texas, Austin, presented lectures at the ERDC MSRC on January 10, 200l, describing recent ideas related to data structures and the use of factory and framework concepts for development and implementation of adaptive mesh finite simulators and for handling multiphysics applications. General concepts were described and contrasted with the "traditional" approach of finite element analysis and software engineering. The design patterns approach was also discussed and examples given. To illustrate several key ideas in the adaptive mesh refinement context, a TESTbed factory and representative results were introduced. Implications for wide application of these ideas were discussed and then the extension of this approach to three-dimensional Parallel Finite Element Framework. An important part of a Framework for DoD applications is the ability to handle multiphysics interoperation. Also considered was the problem of interfacing mesh generators like CUBIT and dynamic repartitioners like ZOLTAN.

Dr. Robert T. McLay, University of Texas, Austin, shown with Bob Athow, ERDC MSRC PET Government Lead

Strategic Planning 2001 Workshop

A strategic planning workshop for the ERDC MSRC was held in Vicksburg, Mississippi, late January and early February 2001 to discuss goals and envision possible accomplishments for the next 5 years for the ERDC MSRC.

Alcorn State University students, March 20, 2001, Wayne Jones (far left), ITL, and Dennis Gilman (far right), ERDC MSRC

Brad Comes (left), ERDC MSRC Director, and COL Gary Royster (right), Director, Intelligence Policy, Office of the Deputy Chief of Staff for Intelligence, The Pentagon, March 9, 2001

WARPLEX participants, February 6, 2001, in the Collaboratorium, ERDC ITL

Members of the Command Staff Inspection Team, Headquarters, U.S. Army Corps of Engineers,with Brad Comes, ERDC MSRC Director, March 8, 2001

Leadership Vicksburg participants, February 6, 2001, Dr. Lisa Hubbard (far left), ERDC Coastal and Hydraulics Laboratory

Continued on page 34

New Leadership
for the ERDC MSRC

by Rose J. Dykes

Exciting new leadership for the ERDC MSRC inspires its personnel to regard each new challenge as an opportunity to continue learning and to imagine that unlimited accomplishments can be made with the potential teamwork of its organization along with its users and associates. Competent and caring new leaders energize motivation and offer encouragement and support.

New leadership for the ERDC MSRC begins with the President of the United States. Although the President is far removed from the MSRC, the top office in the country has a definite impact. George W. Bush was elected the 43rd President of the United States and proposes to strengthen the military with “better pay, better planning, and better equipment.” New Vice President Richard B. Cheney earned the respect of Americans while serving as Secretary of Defense with his direction of two large military campaigns—Operation Just Cause in Panama and Operation Desert Storm in the Middle East. He served three Presidents and as an elected official before his election as Vice President.

The new Chief of Engineers at Headquarters, U.S. Army Corps of Engineers, LTG Robert B. Flowers, shares a consistent vision with that of ERDC and the ERDC MSRC. His visits to the ERDC headquarters in Vicksburg, Mississippi, and personal messages reinforce the ERDC vision and strategy. He expressed his philosophy in a video message to all ERDC employees saying “first understand, then seek win-win solutions.” A “permission slip” signed by General Flowers was presented to each employee following the video presentation.

Less than a year ago, Dr. James R. Houston became the first Director of ERDC. The U.S. Army Engineer Waterways Experiment Station (WES) is now the site of the ERDC command headquarters. Dr. Houston expressed his support of HPC as follows: “High performance computing is very important to the Corps of Engineers, the Army, and the DoD to ensure that the U.S. warfighter has the advantage on the battlefield of the future. The ERDC MSRC, located in the ERDC Information Technology Laboratory, plays a major role in helping us provide this advantage.”

The DoD High Performance Computing Modernization Program (HPCMP), with Cray Henry as its Director, announced a new Deputy Director and a new Chief Scientist. Dr. Larry P. Davis in his new position as Deputy Director of the HPCMP will assist Mr. Henry in managing all Program activities. He will also continue to be responsible for the Program’s requirements and resource allocation activities. This essential process identifies, collects, and validates DoD's high-performance computing requirements and then provides a mechanism for the Services and Defense Agencies to prioritize those requirements in the form of allocations on the Program's HPC systems. Included in the effort is management of the set of DoD Challenge Projects, which represent the largest and highest priority computational work done within DoD's science and technology and test and evaluation communities.

Dr. Davis is a research staff member at the Institute for Defense Analyses. He has been continuously involved with the DoD HPCMP from its inception, originally representing the Air Force on the HPC Working Group that founded the Program. During a 21-year Air Force career that concluded in 1994, Dr. Davis performed research at several Air Force laboratories, taught chemistry at the Air Force Academy, managed the Computational Chemistry Research Program for the Air Force Office of Scientific Research (AFOSR), and served as the Assistant Chief Scientist of Air Force Systems Command (AFSC). He became deeply involved in Air Force HPC activities while at AFOSR and AFSC. Since 1994, he has supported the DoD HPCMP in a number of key areas.

Dr. Davis holds a Ph.D. in physical chemistry from Louisiana State University, an M.S. in systems management from the University of Southern California, and a B.S. in chemical physics from Louisiana State University. He is a member of the American Chemical Society and has published approximately 20 articles in refereed scientific journals.

In his new position as Chief Scientist with the HPCMP, Dr. Frank Mello is responsible for coordinating HPC technical issues between HPC users and the Program's HPC initiatives. Dr. Mello will investigate optimum mapping of DoD HPC users' applications to available HPC architectures. He will examine how efficiently these applications are processed on different architectures and recommend the appropriate mix of HPC capabilities to support the DoD science and technology and test and evaluation missions.

Dr. Mello, a Principal Member of the technical staff at the Department of Energy's (DoE) Sandia National Laboratories joins the HPCMP from the Office of the Director of Operational Test and Evaluation (DOT&E). Within the Live Fire Testing Branch, his duties included oversight of the Live Fire Test and Evaluation (LFT&E) of ballistic missile defense acquisition programs, coordinating the LFT&E sponsorship of the Target Interaction Lethality and Vulnerability Working Group and interfacing between the DoE laboratories and the DOT&E. He represented DOT&E and LFT&E on several Modeling and Simulation working groups dealing with Simulation Based Acquisition, the Simulation Test and Evaluation Process, the Joint models (JMASS, JSIMS, JWARS), and HPC. Dr. Mello has authored numerous publications on computational mechanics.

Dr. Leslie Perkins is the new Project Manager for the CHSSI/PET activities. Dr. Perkins joins the HPCMP from the Air Force Research Laboratory's (AFRL) Propulsion Directorate at Edwards Air Force Base, California. As Assistant Chief Scientist for AFRL-Edwards, her duties included overseeing the basic research efforts—totaling about $2.4 million—conducted at the Edwards' research site. She was also responsible for the final technical review of all in-house and contract programs. She supervised 11 Air Force Palace Knight Program participants and served as Program Element Monitor for basic research activities. Her experience includes administering the National Research Council and AFOSR Summer Research Programs. Over the last 3 years, Dr. Perkins has served as the Computational Chemistry and Materials Science Computational Technology Area Lead for the DoD.

Dr. Perkins holds a Ph.D. in physical chemistry from Iowa State University and a B.S. degree in chemistry from the University of New Orleans. The ERDC MSRC looks forward to Dr. Perkins leading the HPCMP into the future with the follow-on PET Program and the multidisciplinary CHSSI Program.

The ERDC MSRC is pleased with the new leadership in place that will help to ensure that its mission to deliver HPC leadership, service, education, and technical expertise to achieve research and engineering objectives vital to the Nation will be accomplished.


HPC
Modernization Program
High Performance Computing Modernization Program
SC2000
WELCOME
TO SC2000
Simulation of Titan IVB Transonic Buffet Environment
V-22 Osprey Operational Evaluation
Unsteady Aerodynamics of Advanced Guided Munitions
Analysis of Infrared Radiance Effects from Divert Jet Exhaust Flow Over the THAAD Seeker Window
Parallel Simulations of Spray Combustion

New Technology—the Leading Edge at SC2000

by David Stinson

Each year the HPC Modernization Program (HPCMP) participates in SCxy, a large conference where computer hardware and software vendors show off their wares, and universities and research organizations present projects that they have in the works.

During the week of November 4-10, Dallas, Texas, served as the host site for SC2000. SC2000 is sponsored by the Institute of Electrical and Electronics Engineers Computer Society and the Association for Computing Machinery's Special Interest Group on Computer Architecture. The DoD HPCMP has participated in the conference each year since 1994.

New features added to this year's conference included Venture Village, eSCape 2000, a reconfigured HPC Games, Co-Chaired by NAVO MSRC's Eleanor Schroeder, and a new networking award. Venture Village showcased a collection of entrepreneurial information technology companies, all creating new products to build the infrastructure of tomorrow. The eSCape 2000 thrust demonstrated the ability to "escape" from today's technological boundaries and to connect and compute anywhere. Messrs. Stephen Jones and John West, ERDC MSRC, served as Co-Chairs for this event. The SCinet 2000 network showcased leading-edge technology throughout the conference. Dr. Louis Turcotte, formerly of the ERDC MSRC, served as the overall Conference Chair. After presentations of tutorials and the education program over the weekend and through Monday morning, the convention center floor was opened to the public Monday evening with a Gala Opening Reception. The week was laced with talks from invited speakers, presentations of technical papers and awards, panel discussions, and Birds-of-a-Feather sessions.

The DoD HPCMP was well represented. In addition to the many HPCMP persons serving in key leadership and planning roles in the conference, HPC Modernization Program participants presented papers and posters (referred to as Research Gems this year).

Each year, one of the HPCMP MSRCs is responsible for hosting a booth at the conference. This year, the responsibility rested with the ERDC MSRC. Although many hours of hard work were spent preparing for the booth, those participating in the preparation found it a great experience. Only one MSRC is responsible each year for organizing the DoD booth, but the other MSRCs and Distributed Centers provide input in the way of graphics, demonstrations, and booth workers. The experience for all was great—the leading-edge technology exhibited was extraordinary.

SC2000 DoD HPCMP Booth Setup

David Stinson (left), DoD HPCMP Booth Chairman, and Charles Ray (right), ERDC MSRC, pose for a picture as the booth setup is almost complete

(Left to right): Chesley Cuicchi, Kelly Lanier, Jeanie McDonald, and Dean Hampton, all of the ERDC MSRC, practice with the information kiosk before the reception begins

Brad Comes, ERDC MSRC Director, tests the information kiosk

Mike Moore, ASC MSRC, Eleanor Schroeder, Naval Oceanographic Office (NAVO) MSRC, and Dean Hampton, ERDC MSRC

NAVO MSRC group at HPCMP booth (left to right): Bob Knesel, Pete Gruzinskas, Eleanor Schroeder, Christine Cuicchi, and Steve Adamec

David Stinson, DoD HPCMP Booth Chairman, gives instructions to the ERDC MSRC Outreach Team members before the Gala Opening Reception

(Left to right): Dr. Louis Turcotte, Conference Chair, Stephen Jones, eSCape 2000 Co-Chair, and Dr. Dennis Duke, Venture Village Vice Chair

Pete Gruzinskas, NAVO MSRC, Frank Cameron and Rita Wilkey, Naval Air Warfare Center, and Steve Schneller, Naval Undersea Warfare Center

Shown visiting with Dr. Louis Turcotte (center), Conference Chair, in the Research Gems/eScape 2000 area of the conference are (left to right) Charles Ray, Rose Dykes, Chesley Cuicchi, Kelly Lanier, Jeanie McDonald, and Dr. Phu Luong, all of the ERDC MSRC

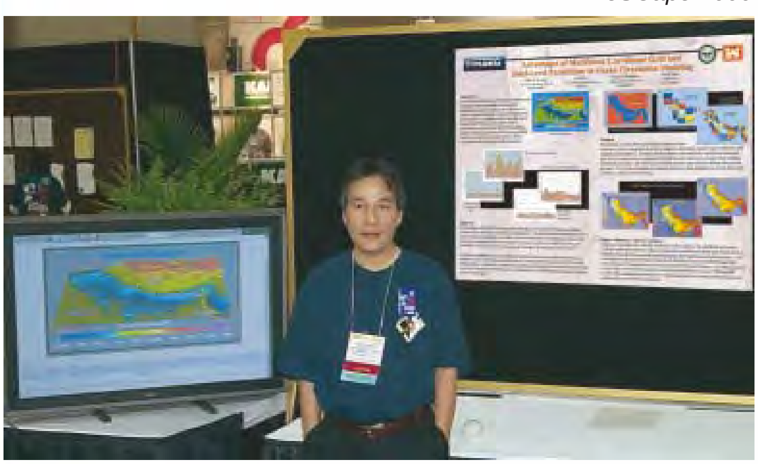
An eScape 2000/Research Gems shirt is donned by someone speaking with Stephen Jones, eScape 2000 Co-Chairman

SCinet 2000 established flexible, wide-area connections to the show floor, installing and operating more than 40 miles of fiber optics throughout the conference areas

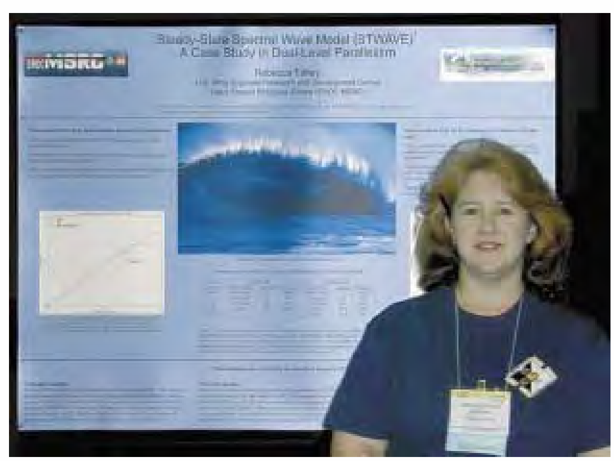
Entrance to Venture Village

Entrance to Research Gems/ eScape 2000

Entrance to SC2000 Convention floor



Dr. Phu Luong, ERDC MSRC, participates in the Research Gems sessions with his poster presentation entitled "Advantages of Multiblock Curvilinear Grid and Dual-Level Parallelisms in Ocean Circulation Modeling"



Rebecca Fahey, ERDC MSRC, and her award-winning poster entitled "Steady-State Spectral Wave Model (STWAVE)—A Case Study in Dual Level Parallelisms"


Jeff Graham and Hank Laughlin, ASC MSRC, along with Dean Hampton, ERDC MSRC


Pete Gruzinskas, NAVO MSRC, demonstrates HPC research projects to a young visitor

Susan Pfeiffer-Vega, HPC Modernization Office, at the HPCMP booth greeter's table

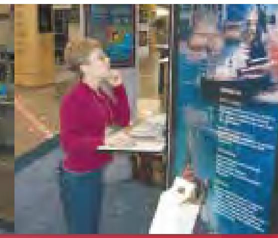

Professor Shahrouz Aliabadi, Clark Atlanta University, views HPC research projects at DoD HPCMP booth

Cathy McDonald, HPC Modernization Office, and Eleanor Schroeder, NAVO MSRC, man booth as Steve Adamec (left), NAVO MSRC Director, and Dr. George Heburn (right), NAVO MSRC, visit


Jay Cliburn, ERDC MSRC, visits at booth with Virginia Bedford, Arctic Region Supercomputing Center







Leading-Edge Technology

SC2000 DoD HPCMP Booth

Charles Ray, ERDC MSRC, Frank Lavoto, NAVO MSRC, and Dennis Gilman, ERDC MSRC

Brad Comes, ERDC MSRC Director, assists in tear down of booth as Pete Gruzinskas, NAVO MSRC, and Charles Ray, ERDC MSRC, watch with some concern

Charles Ray ready with the truck for leaving Dallas

ERDC MSRC group smiles as everything is packed at the end of SC2000
Front row (left to right): Rose Dykes, Dean Hampton, Jeanie McDonald, Kelly Lanier, David Longmire
Second row (left to right): Dana Allen, David Stinson, Chesley Cuicchi, Brad Comes
In back: Charles Ray

Damage Simulations in Hard and Deeply Buried Targets as a Result of Blast and Shock Loading

Dr. G. W. McMahon, B. J. Armstrong, Jr., and C. E. Joachim

The counterproliferation of weapons of mass destruction (WMD) continues to remain one of the Nation's highest defense priorities. The defeat of systems within hard and deeply buried targets, namely tunnels, presents the greatest challenge. When a weapon detonates in a confined area, the airblast effects are much more severe than those from a free-air detonation. The size and complexity of numerical models required to assess functional damage to a facility require HPC resources.

The geometries of hard and deeply buried targets in rock range from long straight tunnels to complex geometries with multiple levels. Substantial HPC resources are required for an accurate numerical model representation of the complex three-dimensional (3-D) geometry and functional layout, the interaction of the blast wave with mission-critical and support equipment, and the response of the equipment to failure.

Computer Codes used in Numerical Modeling: Blast environments were simulated using the scalable hydrodynamic code CTH. The equipment response was simulated with a parallel version of DYNA (ParaDyn), a finite element code. The calculations were conducted on the ERDC MSRC Cray T3E, IBM SP, and SGI Origin 2000. The calculations involve modeling high-explosive initiation and detonation effects, large deformations, and damage. The problems are also 3-D and involve complex interactions with objects in the blast flow. CTH [1] and ParaDyn [2] are multidimensional scalable computer codes widely used in the defense research and development community to model shock physics and large deformation problems. CTH is a finite volume-based, explicit time integration method and uses Eulerian formulations. ParaDyn is a rate-based, finite-element, explicit time integration method and uses Lagrangian formulations.

Airblast Simulation: Ideally, the entire calculation—from the initiation of a charge, blast propagation, interaction of the blast wave with the equipment, and equipment response—should be conducted in three dimensions as a single, coupled calculation. Limits to computational resources require that approximations be made to the geometry in order to reduce the calculation size. Since the environment calculation must be decoupled from the loading and equipment response, only limited aspects of the problem can be simulated in a detailed 3-D grid. For the tunnel geometry in Figure 1, the differences in problem size and the computational resources required for these two approaches are given in Table 1. If the tunnel geometry is represented as a planar 2-D structure, the localized charge has to be distributed so that the mass of the distributed charge equals the mass of the concentrated charge (Figure 2). The 2-D calculation results for this tunnel are compared with results from a 3-D calculation in Figure 3. The 3-D calculation waveforms are compared with experimental data in Figure 4. Figures 5 and 6 show the blast wave propagation down the tunnel before and after engulfment of the storage tank. The reflected shock from the back wall and the multiple shock reflections from the alcove are evident in the waveforms.

Table 1
Comparison of Computational Resources for 2-D and 3-D Tunnel Airblast Calculations

Resource	2-D Calculation	3-D Calculation
Machine	IBM SP	T3E
Processors	96	256
Code	Parallel CTH	Parallel CTH
Grid Size	0.8 million cells	33 million cells
Minimum Cell Size	50.0 mm	60.0 mm
Width of Grid	80 meters	80 meters
Height of Grid	25 meters	25 meters
Memory Size	6.5 MBytes	12 GBytes
Average File Dump Size	160 MBytes	65 GBytes
Run Time	1,000 cpu hours	25,000 cpu hours

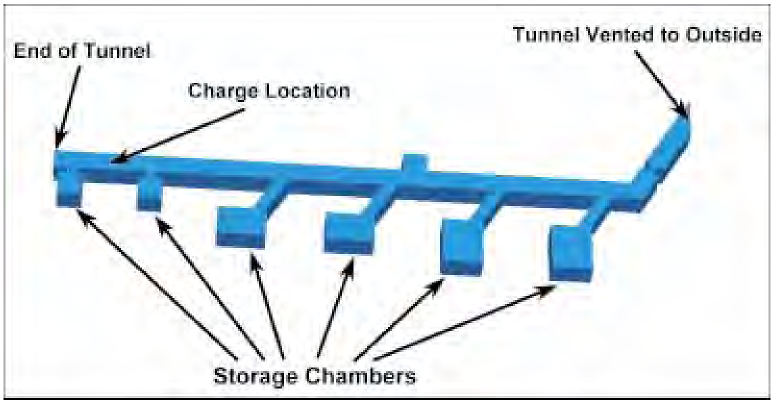


Figure 1. Full-scale tunnel layout

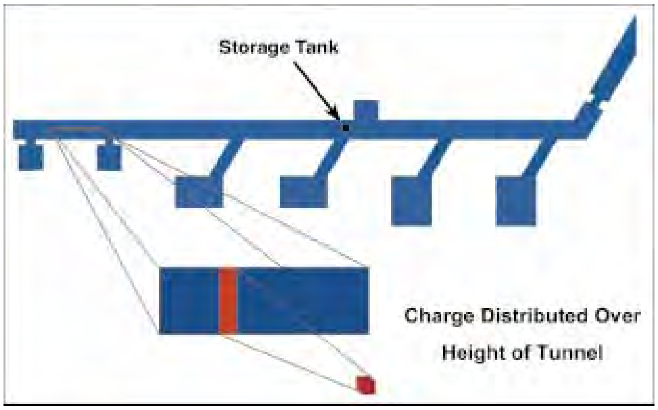


Figure 2. Two-dimensional planar model of tunnel

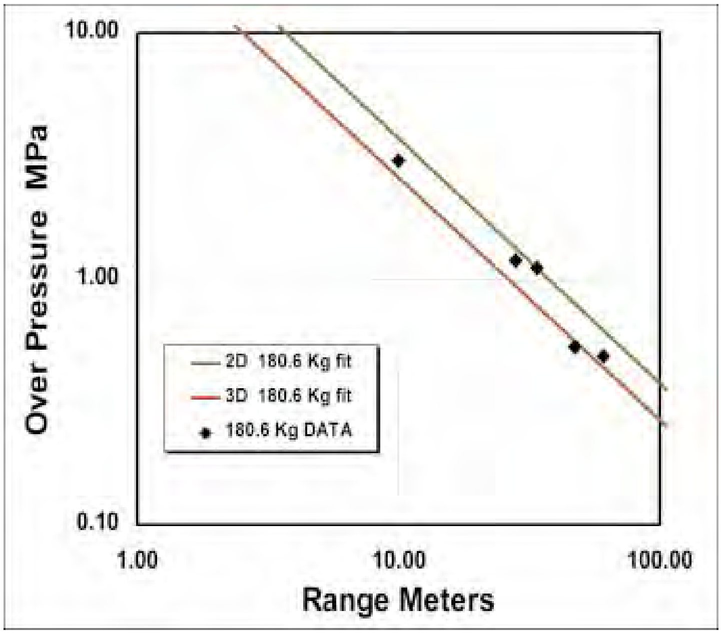


Figure 3. Comparison of pressure versus range from CTH 2-D and 3-D calculations

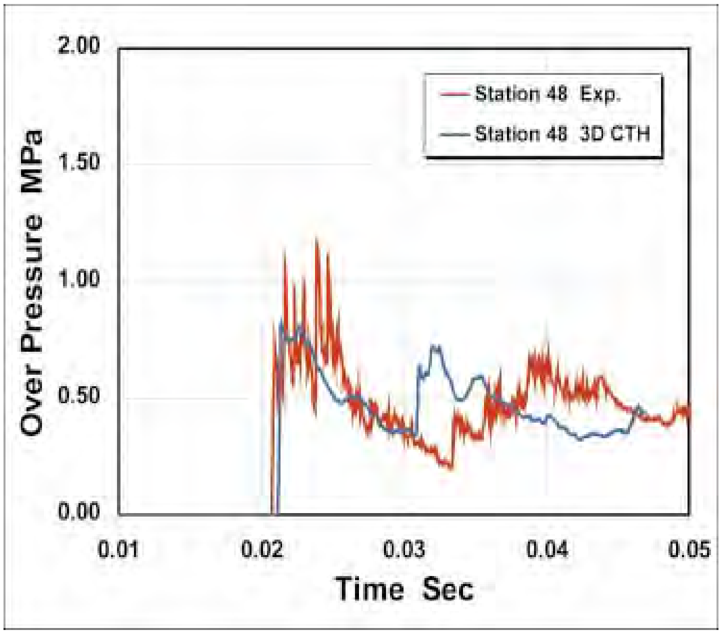


Figure 4. Comparison of pressure history from 3-D model with test results

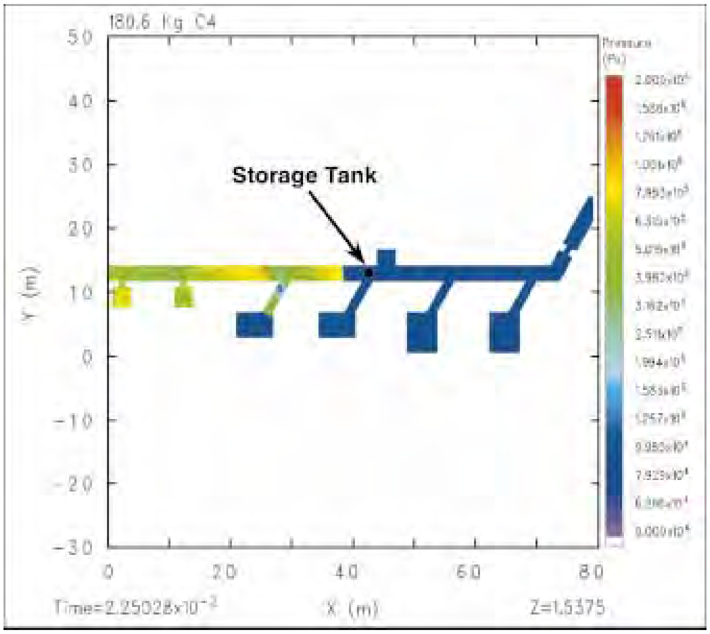


Figure 5. Blast wave propagation from 3-D calculations in tunnel before engulfment of storage tank

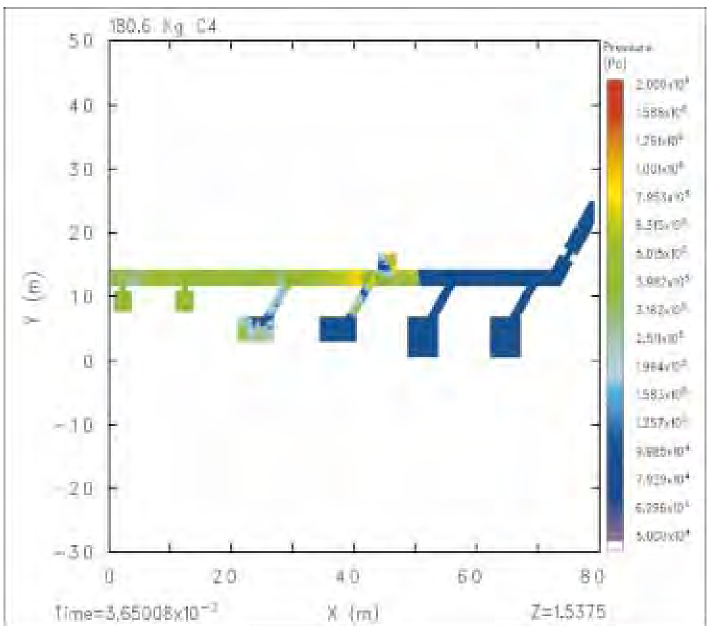


Figure 6. Blast wave propagation from 3-D calculations in tunnel after engulfment of storage tank

Equipment Loading and Response: In these calculations, the storage tank is modeled as a solid steel structure. Assuming that the tank is a solid, rigid structure, any modification of the load on the structure that would result from interaction of the airblast with an actual deforming structure is lost. However, these losses are considered small, as the tank orientation does not change significantly during engulfment. The loads calculated on the 2- and 3-D solid structure are applied to a 3-D finite element representation of the tank. Comparisons of test results with calculations for the tank response are shown in Figure 7.

Discussion of Results: The discrepancy between the 2-D numerical simulation and the experiment appears to be the result of the planar approximation in which a concentrated charge is simulated with one that is distributed across the cross section of the tunnel. The 3-D calculation of the detonation and airblast propagation reproduced the shock arrival and the incident shock strength quite accurately. The arrival of the reflections in the calculation is not consistent with the data and is the result of the reflection from the back wall and multiple shock interactions at the airblast gauge location at Station 48. The response of the tank was overpredicted; but at this level of response, small variations in the load can lead to large increases in response. Overall, the 2-D planar approximations appear to lead to unacceptable results, and problems of this type will have to be addressed by 3-D calculations. Even with the large computing resources that would be required, using 3-D numerical models is much more cost effective than conducting full-scale experiments. In the near future, the plans are to validate coupled Eulearian/Lagrangian codes against this class of problems.

Acknowledgments

Permission from Headquarters, U.S. Army Corps of Engineers, to publish this article is gratefully acknowledged. The assistance of Dr. J. P. Balsara, Ms. Sharon B. Garner, and Mr. L. K. Davis is greatly appreciated.

References

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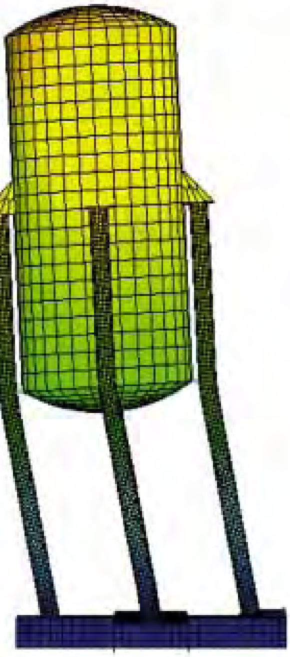
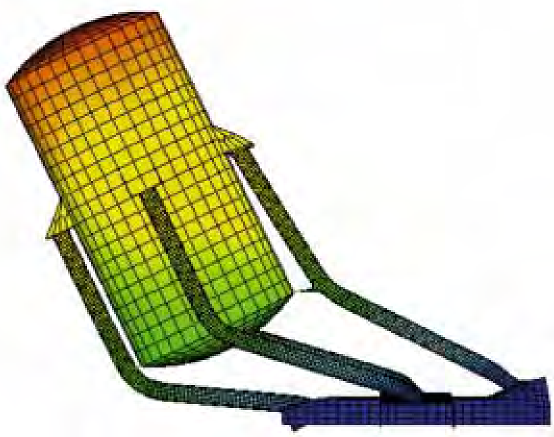
2. Hoover, C.G., DeGroot, A.J., Maltby, J.D., and Procassini, R.J., “ParaDyn: DYNA3D for Massively Parallel Computers,” UCRL 53868-94, Lawrence Livermore National Laboratory, Livermore, CA, 1995.

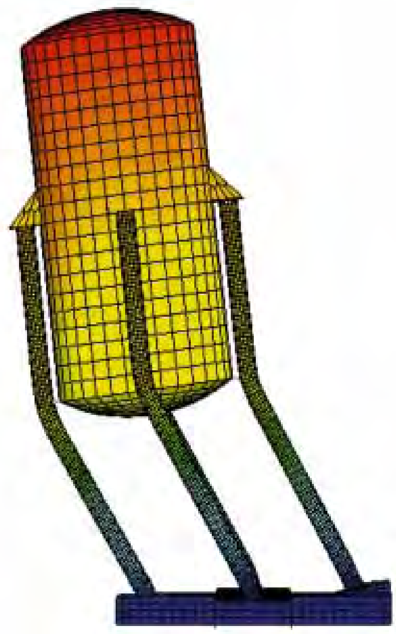
a. Experimental result



b. 3-D finite-element grid with experimental load



c. 3-D finite-element grid with 2-D load



d. 3-D finite-element grid with 3-D load

Figure 7. Calculated (with loads from CTH) and experimental response of storage tank

Dr. McMahon and Mr. Joachim are research civil engineers, and Mr. Armstrong is a research physicist in the Geotechnical and Structures Laboratory at the U.S. Army Engineer Research and Development Center in Vicksburg, Mississippi.

Fifth Annual ERDC MSRC PET Review

Robert F. Athow

February 28, 2001, saw the Fifth Annual ERDC MSRC Programming Environment and Training (PET) Review draw to a close. The PET partners presented a broad spectrum of timely reviews of their support and projects to the HPC community. While torrential rain sought to dampen the presentations, the quality of the products and projects brightened the outside gloom.

(Left to right): Brad Comes, ERDC MSRC Director; Bob Athow, Government PET Lead; Professor Shahrouz Aliabadi, Clark Atlanta University; John Mauldin, CSC Deputy Program Manager

Surprise recognition was given to Professor Emeritus Wayne Mastin for his dedicated service to the ERDC MSRC PET Program. The ERDC MSRC Director, Brad Comes, and the ERDC MSRC Government PET Lead, Robert (Bob) Athow, presented a special commendatory plaque to him.

(Left to right): Dr. Jeffery Holland, Government CTA Lead for EQM; Dr. Phu Luong, EQM Onsite Lead; Professor Mary Wheeler, University of Texas, Austin; Professor Bharat Soni, Mississippi State University; Professor Joe Thompson, Academic Team Lead, Mississippi State University; Brad Comes, ERDC MSRC Director

The newest personnel to the PET Program were introduced to the assembly: Dr. Leslie Perkins, Common High Performance Computing Software Support Initiative (CHSSI)/PET Project Manager for the HPCMP; John E. West, ERDC MSRC Onsite PET Director and Director of Scientific Computing; and Mr. Athow. Brief introductory remarks were made by each of them.

Environmental Quality Modeling and Simulation (EQM) activities were highlighted by Professor Mary F. Wheeler, University of Texas, Austin, and included improving the parallel performance of environmental quality models, full two-dimensional (2-D) parallel implementation of CH3D-Z, interpolation and projection between arbitrary space/time grids, and reactive transport

Front table (Left to right): Professor Joe Thompson, Academic Team Lead, Mississippi State University; Doug Walker, CSC Program Manager; Dr. Leslie Perkins, CHSSI/PET Project Manager, HPCMP; Bob Athow, Government PET Lead; Brad Comes, ERDC MSRC Director; and John West, ERDC MSRC PET Director

(Left to right): Brad Comes, ERDC MSRC Director; Dr. Leslie Perkins, CHSSI/PET Project Manager, HPCMP; Bob Athow, Government PET Lead

schemes for water quality modeling on unstructured grids. A Climate, Weather, and Ocean Modeling and Simulation (CWO) scientific visualization demonstration by Dr. Phu Luong, ERDC MSRC, was particularly interesting to the attendees. Professor Clint Dawson, also from the University of Texas, provided insights to his work.

Commendatory plaque was presented to Professor Emeritus Wayne Mastin for his service to the ERDC MSRC PET Program. (Left to right): Bob Athow, Brad Comes, Professor Mastin, John West, Professor Joe Thompson

Specific EQM projects addressing parallel implementation issues relating to the groundwater contaminant transport code FEMWATER were presented by Professors Tom McGehee and Mike McAdams of Texas A&M University, Kingsville.

Professor Graham Carey and Dr. David Littlefield, University of Texas, Austin, and Dr. Richard A. Weed, ERDC MSRC, presented the Computational Structural Mechanics (CSM) core support and project activities. Algorithm enhancements, adaptive mesh technology and mesh improvement for hypervelocity impact and penetration analysis, discontinuous Galerkin FE and adaptive grids, error and feature indication in interpolation and approximation algorithms, and hierarchical data mining of very large data sets for remote visualization and manipulation were all presented.

Professor Shahrouz Aliabadi, Clark Atlanta University, discusses parallel simulation of waves interacting with marine vessels in motion

Professor Bharat Soni, Mississippi State University, and Dr. Nathan Prewitt, ERDC MSRC, presented the work within the Computational Fluid Dynamics (CFD) core support and project sphere including grid assembly enhancements for Chimera technology, JAVA-based CFD training tools, and a library of interpolation and approximation models (INLiB). Professor Shahrouz Aliabadi, Clark Atlanta University, addressed two projects, parallel simulation of wave interacting with marine vessels in motion and parallel remote visualization. He also showed a one-billion tetrahedral unstructured element mesh application with a sustained speed of over 230 gigaflops on a Cray T3E with 1,088 processing elements.

(Left to right): Beverly Bradley and Eigoro Hashimoto, Naval Oceanographic Office, shown with Kelly Lanier, PET Training Coordinator

(Left to right): Professor Keith Bedford and Dr. David Welch, Ohio State University, and Dr. Stephen Wornom, CWO Onsite Lead

Professor Keith Bedford and Dr. David Welsh, Ohio State University, and Dr. Stephen Wornom, CWO Onsite Lead, presented the Climate, Weather, and Ocean Modeling and Simulation activities, which included application of SWAN and the coupling of wave-current-sediment models (COMAPS) for nearshore and tributary plume predictions.


(Left to right): Dr. Jeffery Holland, Government CTA Lead for EQM; Dr. Phu Luong, EQM Onsite Lead; and Professor Clint Dawson, University of Texas, Austin

Collaboratory actions were the focus of the presentations by Dr. Polly Baker, University of Illinois, in Scientific Visualization, Dr. Wojtek Furmanski, Syracuse University, with the FMS SPEEDES installation and training, and Professor Geoffrey C. Fox, Florida State University, communication/collaboration with modular collaborative environments.

Scalable Parallel Processing Tools presentations were made by Dr. Richard Hanson, Rice University, Professor Behrooz Shirazi, University of Texas, Arlington, and Dr. David Cronk, University of Tennessee. Support for PARSA using fortran pthreads and the SARA-3D structural technology acoustics applications were all of interest.


Dr. Polly Baker, University of Illinois, shown with Professors David Littlefield and Graham Carey, University of Texas

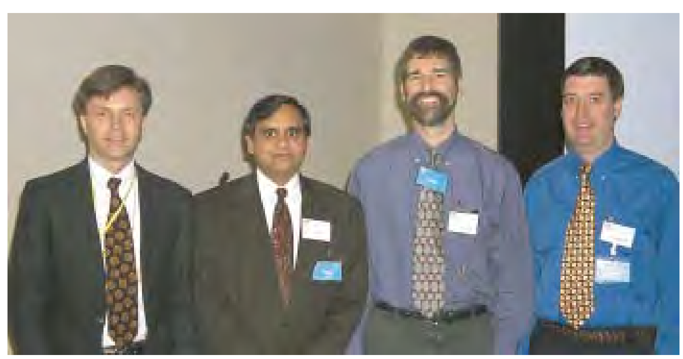
All presenters focused on their continued efforts in training users, both onsite and remotely. Professor Mastin specifically highlighted the ERDC MSRC's onsite training activities. The summer intern program at Clark Atlanta University and the classes with Jackson State University were given particular credence.

The overriding success of this annual meeting is best illustrated by the many formal and informal interactions and collaborations that crosscut all the computational technology areas. And it was fun and interesting too!


(Left to right): Dr. Nathan Prewitt, CDF Onsite Lead, visits with Dr. Ralph Noack, Army Research Laboratory


(Left to right): Bob Athow, Government PET Lead; Professor Joe Thompson, Academic Team Lead, Mississippi State University; John West, ERDC MSRC PET Director


(Left to right): Professors Jeff Marquis and Behrooz Shirazi, University of Texas, Arlington, and Dr. Richard Hanson, Rice University


(Left to right): Dr. Nathan Prewitt, CFD Onsite Lead; Professor Bharat Soni, Mississippi State University; Dr. Ralph Noack, Army Research Laboratory; Hugh Thornburg, Aeronautical Systems Center MSRC

Shown visiting between presentations (left to right): Dr. Jeffery Holland, Government CTA Lead for EQM; Brad Comes, ERDC MSRC Director; and Professor Bharat Soni, Mississippi State University

(Left to right): Professor Mary Wheeler, University of Texas, Austin, and Dr. Fred Tracy, ERDC Scientific Advisor for PET

Professor Keith Bedford, Ohio State University, discussed CWO core support—onsite and offsite

Professor Behrooz Shirazi, University of Texas, Arlington, and Dr. Nathan Prewitt, CFD Onsite Lead

Professors Behrooz Shirazi and Jeff Marquis, University of Texas, Arlington

(Left to right): Professors Wojtek Furmanski, Syracuse University and Geoffrey Fox, Florida State University

Professor Mary Wheeler, University of Texas, and Professor Joe Thompson, Mississippi State University

Dr. Robert Hall, ERDC Geotechnical and Structures Laboratory, and Dr. Rick Weed, CSM Onsite Lead

(Left to right): Dr. Phu Luong, EQM Onsite Lead; Professor Clint Dawson, Dr. Lea Jenkins, and Professor Mary Wheeler, University of Texas, Austin

IBM SP Switch2

Jay Cliburn

Recently, the ERDC MSRC upgraded the interconnection fabric of the IBM Power3 symmetric multiprocessor (SMP) machine called “Cobalt.” The new interconnection switch is known as the *SP Switch2*. Cobalt consists of 64 nodes containing eight processors each, for a total of 512 central processor units (CPUs). Each node runs its own copy of the AIX operating system.

The interconnection fabric that binds the individual nodes into a cooperative whole is called the *SP Switch*, or simply “the switch.” Whenever a parallel process needs to pass information to a cooperating process on another node, the information is passed over the switch. The specific mechanism employed by each process to effect the information transfer is called a *switch window*. Switch windows are assigned to processes at job start-up time.

Prior to the switch upgrade, any given Cobalt node could support a maximum of four switch windows, thus imposing an upper limit of four simultaneous message-passing interface (MPI) or serial processes, even though each node contains eight CPUs. The switch window deficit was eliminated with the installation of the SP Switch2. There are now sixteen switch windows available per node; one for each of the eight CPUs plus a surplus of eight windows for future growth.

The SP Switch2 enables full utilization of the installed 8-way nodes, higher job densities, and more efficient placement of jobs on the ERDC MSRC Power3 SMP machine, resulting in lower overall job queue wait times for user jobs. The ERDC MSRC is excited to offer this increased capability to its customers.

ERDC MSRC Network Status

Michael Nassour

The bandwidth capacity of the Internal Major Shared Resource Center (MSRC) Network (IMN) has changed very little since 1996. The current backbone technology, Fiber Distributed Data Interface (FDDI), with a theoretical transfer rate of 100 Mbps (Megabits per second), experiences sustained utilization of more than 40 percent with peak utilization at or near 100 percent. In contrast, the network capability of the computing systems within the MSRC, as well as the data movement requirements of the user community, has steadily increased. Recent initiatives for sharing and storing data have significantly increased the backbone infrastructure capability within the MSRC.

The two most noticeable improvements to the IMN were converting the interactive FDDI-accessed systems to ATM OC-12c (622 Mbps) interfaces and implementing a Gigabit Ethernet (1,000 Mbps) backbone for internal data transfers. The Defense Research and Engineering Network (DREN) users should notice a drastic improvement in interactive connectivity, as many intermediate translation devices have been removed; i.e., OC-12 from DREN to FDDI interactive became a direct OC-12 “pipe” from DREN to the HPC system. The larger “pipe” provides numerous opportunities for inter-MSRC initiatives such as metacomputing.

The upgrades were implemented in the most transparent way possible to the users by using a domain name system (DNS) to resolve host names. If one used host entries in local configuration files, changes to the setup were required to address the new network infrastructure.

Grid Computing Development

Greg Rottman

Development of grid computing technology continues. Greg Rottman attended the Grid Forum meeting held in Boston on October 15-18, 2000. The Grid Forum is a voluntary organization that helps create grid technologies and interoperability while reducing duplicated efforts. Greg also represents the ERDC MSRC on the MSRC Metacomputing Working Group (MCWG). The MCWG has representatives from across the program that work to promote the development of computational grid technology across all the centers. Greg continues to work closely with the MCWG to develop a plan for the initialization of a project to create a computational grid for the HPCMP.

New Origin 3800 System

Rebecca Fahey

The ERDC MSRC is pleased to announce its newest high-performance computer, an SGI Origin 3800 (O3K), which replaced an SGI Origin 2800 system (O2K). The new system was initially four 128-processor images that ultimately became a single 512-processor image. This new system provides eight times the computing power of the old SGI Origin 2000 system it replaced.

The new Origin system offers a number of improvements over the old system. The processors on the new O3K are more than twice as fast as the processors on the old Origin system, with 400-MHz processors as compared with 195 MHz. This increase in processor speed resulted in the expected two-times speedup for most of the codes tested on the system. A few codes exhibited even greater speedup that was attributed to general system design improvements. The new system also offers two times the per-processor memory offered by the old system, with an aggregate total of 512 GB.

The new O3K also has four times the number of processors as the O2K. The process of combining the four 128-processor images occured in stages. In this first stage, the four 128-processor images were combined into two 256-processor images. This increased the maximum number of processors that can be used by a single job to 256. In the final stage, the two 256-processor images were combined into a single 512-processor image, allowing a single job to utilize as many as 512 processors.

The extra processors, increased processor speed, and increased memory of the new O3K system have been a welcome improvement. Users are now able to run larger jobs, utilize more processors, and enjoy a faster turnaround time on their jobs. With these improvements, the Origin problem size and user base is expected to increase significantly. If one has been considering a move to an Origin machine, this may be a good time to make the transition. To obtain additional information about the new SGI Origin 3800 system, refer to the Web site at *www.wes.hpc.mil* or contact the Customer Assistance Center at 1-800-500-4722.

technology update

Mass Storage Facility Utilities

Drs. Mark R. Fahey and Thomas Oppe

The ERDC MSRC has several commands for manipulating files on the Mass Storage Facility (MSF). These commands are available on all HPC hosts, as are man pages for each command.

Note that there are two "MSF" machines: new and old, for lack of better naming convention. Whenever the MSF utilities are used to store files, the files are stored on the new MSF. However, if you telnet or ftp to msf, you will be logged into the old MSF.

To put files on the (new) MSF, the commands `msfput` and `msfmput` are available. The basic usage of these two commands is as follows:

```
msfput local-file [remote-file]
msfmput [-d remote-path] local-files
```

Note that for the multiple put, the remote path comes first, then the local files to be moved.

Once the files are on the (new) MSF, the files can be manipulated just like the files in your own homespace using MSF utilities. Commands for manipulating files already on the MSF are as follows:

`msfchmod -m mode files`, where -m mode specifies the permissions to be given

```
msfls [-o] files
msfmkdir [-o] remote-dir
msfmv [-o] remote-file target-file
msfrm [-o] files
msfrmdir [-o] remote-dir
```

where `-o` forces the utility to perform its action on the old MSF.

There is one utility that checks the status and availability of the MSF:

```
msfstat [-o]
```

For files already on the MSF (new or old), two routines are used to retrieve files:

```
msfget remote-file
msfmget [-d path] remote-files
```

Note that just the like the msfmput, the remote path must be specified first.

There are also two commands for copying files from the old MSF to the new MSF:

```
msfcopy remote-file
msfmcopy [-d path] remote-files
```

See the man pages for more information and options about each function.

Origin 3000 versus 2000...A Few Tips

Drs. Mark R. Fahey and Thomas Oppe

The ERDC MSRC has installed a new SGI Origin 3800. This machine replaced the Origin 2800. Many users had grown accustomed to the Origin 2800 and will have to learn a few new things to run on the Origin 3800.

New qsub option

First, when submitting batch jobs on the 2800, the option ncpus was used to specify the number of processors. On the 3800, this option is not used nor accepted by PBS. The correct syntax for specifying the number of CPUs on the 3800 is

```
-lnodes=1:ppn=#
```

where # is the desired number of CPUs. When the system first went on-line, the maximum value for ppn was 128. The maximum possible value is now 512. Note that 1 is the only acceptable numeric value for "nodes=1".

SCS Library

Another difference many users will encounter is the name of the SGI scientific library. The SGI scientific library was well known to be named COMPLIB or COMPLIB.SGIMATH. However, the name of the new scientific library is SCSL.

The SGI scientific library (SCSL) is a collection of high-performance scientific libraries that provide support for mathematical and numerical techniques used in scientific computing.

To get more information about the SCSL library, type "`man intro_libscsl`" or "`man intro_scsl`".

A very important difference between COMPLIB.SGIMATH and SCSL is that COMPLIB has the old LINPACK and EISPACK routines in addition to the LAPACK routines, but SCSL does not. Thus, users will have to either port their LINPACK and EISPACK calls to LAPACK calls or obtain the EISPACK and/or LINPACK routines they need.

The following sublibraries are included in the current release of SCSL:

- Signal processing routines
  - Fast Fourier Transform (FFT) routines
  - Convolution routines
  - Correlation routines
- Linear equation solvers for sparse systems with symmetric nonzero structure
- Vector-vector linear algebra subprograms
  - Level 1 Basic Linear Algebra Subprograms (Level 1 BLAS)
- Matrix-vector linear algebra subprograms
  - Level 2 Basic Linear Algebra Subprograms (Level 2 BLAS)
- Matrix-matrix linear algebra subprograms
  - Level 3 Basic Linear Algebra Subprograms (Level 3 BLAS)
- LAPACK, a public-domain software library that solves problems frequently encountered in numerical linear algebra

SCSL is available in 64-bit and 32-bit (n32) modes for the MIPS4 instruction set extensions. To use the SCSL routines, load the library with the `-lscs` or `-lscs_mp` option. The `-lscs_mp` option directs the linker to use the multiprocessor version of the library.

When linking to SCSL with `-lscs` or `-lscs_mp`, the default integer size is 4 bytes (32 bits). Another version of SCSL is available in which integers are 8 bytes (64 bits). This version allows the user access to larger memory sizes and helps when porting legacy Cray codes. It can be loaded by using the `-lscs_i8` option or the `-lscs_i8_mp` option. A program may use only one of the two versions; 4-byte integer and 8-byte integer library calls cannot be mixed.

Furthermore, the SCSL library has new FFT routines. The following table shows FFT routines from the COMPLIB.SGIMATH library and their corresponding routine in the new SCSL library. The routines in the SCSL library can be used to do both initialization and FFT computations.

```
 Complib                      SCSL
------------------         ---------
 cfft1di+cfft1d       ->    ccfft
 cfftm1di+cfftm1d     ->    ccfftm
 cfft2di+cfft2d       ->    ccfft2d
 cfft3di+cfft3d       ->    ccfft3d
```

Modules

A very significant change from the 2800 to the 3800 configuration is the use of modules. Often in the course of tracking down a computer bug, using an earlier version of a compiler or library is helpful. The Modules package on the new SGI 3800 platform is a convenient way for the user to select a different version of software without going to the trouble of modifying his PATH, MANPATH, and other environment variables directly. Modules do this automatically.

First, the "`module list`" command can be used to determine what versions of commonly used software are currently being used:

```
ruby> module list
```

Currently Loaded Module files:

1) modules	3) MPT.1.4.0.2
2) MIPSpro.7.3.1.1	4) SCSL.1.3.0.0

The "MIPSpro" module indicates the version of compilers and basic libraries, while "MPT" (for "Message Passing Toolkit") indicates the MPI and PVM message-passing libraries, and "SCSL" indicates the SGI scientific library containing the BLAS, LAPACK, and other routines. To determine the list of available modules on the system, type "`module avail`":

```
ruby> module avail
----- /opt/modulefiles -----
MIPSpro.7.2.1   MIPSpro.7.3.1.1     MPT.1.4         SCSL.1.3.0.0
MIPSpro.7.3     MIPSpro.7.3.1.2     MPT.1.4.0.2
```

Thus, if the user wishes to select another version of the compiler, the "module switch" command can be used to select an earlier version of the compiler:

```
module switch MIPSpro.7.3.1.1 MIPSpro.7.2.1
```

This switching action can also be accomplished in two steps with

```
module unload MIPSpro.7.3.1.1
module load MIPSpro.7.2.1
```

Note that the term "load" does not indicate that a particular library will be searched automatically; it simply determines which version of the library will be searched. The user must still use "`-lmpi`", "`-lscs`", "`-lscs_mp`", etc., on the linking step to satisfy external references.

To determine where a particular library is located, the "module display <module_name>" can be used. This command will display how the user's PATH and MANPATH variables are altered to access a particular version:

```
ruby> module display SCSL.1.3.0.0
--------------------------------------
/opt/modulefiles/SCSL.1.3.0.0:
Setenv  SCSL_SGI to /opt/scsl/1.3
Prepend /opt/scsl/1.3/usr/lib32 to LD_LIBRARYN32_PATH
Prepend /opt/scsl/1.3/usr/lib64 to LD_LIBRARY64_PATH
Prepend /opt/scsl/1.3/usr/lib32/mips4 to LD_LIBRARYN32_PATH
Prepend /opt/scsl/1.3/usr/lib64/mips4 to LD_LIBRARY64_PATH
Prepend /opt/scsl/1.3/usr/include to INCLUDE_PATH_SGI
Prepend /opt/scsl/1.3/usr/bin to PATH
Prepend /opt/MIPSpro/bin to PATH
Append  /usr/share/catman:/usr/share/man:/usr/catman:/usr/man to MANPATH
Prepend /opt/scsl/1.3/usr/share/catman to MANPATH
--------------------------------------
```

Finally, if the user forgets a "module" keyword, a list is given in response to "`module help`". "`man module`" gives the man page for the modules package. The most commonly used commands are as follows:

`module list` — list all currently loaded modules
`module avail` — list all available modules on the system
module load (or add) <module_name(s)> — load one or more modules
module unload (or rm) <module_name(s)> — unload one or more modules
module switch (or swap) <module_1> <module_2> — replace <module_1> with <module_2>
module display <module_name(s)> — determine how one or more modules are accessed through changes to PATH and MANPATH
`module help` — lists all module keywords

ERDC MSRC Scientific Visualization Center Update

Paul Adams

The Scientific Visualization Center (SVC) team works with scientists and engineers on projects to merge scientific data with computer graphics to enable researchers to perform visual investigations of their data. These visualizations enable a broader understanding of the technical data presented. Using state-of-the-art techniques and equipment, the interdisciplinary team works closely with a wide variety of groups to provide visual clarification on various studies.

One of the current Challenge Projects on the ERDC MSRC systems is the AirBorne Laser II (ABL) project. The problem being studied is that of turbulence in the atmosphere distorting a laser beam as it travels to the target. One portion of the ABL II project deals with these distorting effects of the atmosphere by computationally modeling and simulating earth's upper troposphere and lower stratosphere. Currently, the direct numerical simulation of stratified shear turbulence and gravity-wave breaking runs on 500 CPUs on the ERDC MSRC T3E and produces over 400 GBytes of data from each run. Reducing that data to more understandable information is the challenge facing the ABL project and the SVC team. Figure 1 shows the viscous dissipation of the breakdown of a Kelvin-Helmoltz (KH) vortex caused by stratified shear flow. Figure 2 shows thermal dissipation caused by this same breakdown. The areas of greatest dissipation, both viscous and thermal, are colored in red. The areas of zero dissipation, both viscous and thermal, are colored in black. The regions with the largest values of the thermal dissipation have the greatest impact on the optical properties of the atmosphere through which the laser beam will travel because of the index of refraction's sensitivity to thermal gradients. In other words, it is in these regions that the high-power laser beam will be distorted and defocused before reaching its intended target.

Figures 1 and 2 were created using scientific visualization package OGLE written by Dr. Michael Gourlay.

A second Challenge Project at the SVC is called the Active Control of Fuel Injectors in Full-Scale Gas Turbine Engines. The impetus is to achieve significant improvement in the performance of next-generation gas turbine engines in order to develop lightweight, compact, fuel-efficient propulsion systems for helicopters and tanks for the Army. A reduction in fuel consumption would be beneficial by extending the range of vehicles as well as by reducing the logistical burden of transporting fuel. Experimentally investigating such systems is difficult because of the difficulty in obtaining access to the hot, turbulent, reacting region in the combustor. Figure 3 shows the flame (in yellow) being distorted by a vortex ring (in blue) in the combustion chamber.

Another initiative developed by the SVC team was recently shown at SuperComputing 2000 (SC2000). An interactive DVD was created highlighting the HPCMP. Included on this DVD were videos from the four MSRCs, as well as information from the Distributed Centers, CHSSI Projects, and Challenge Projects. The use of DVD technology is anticipated to play a significant role in future scientific visualization capabilities.

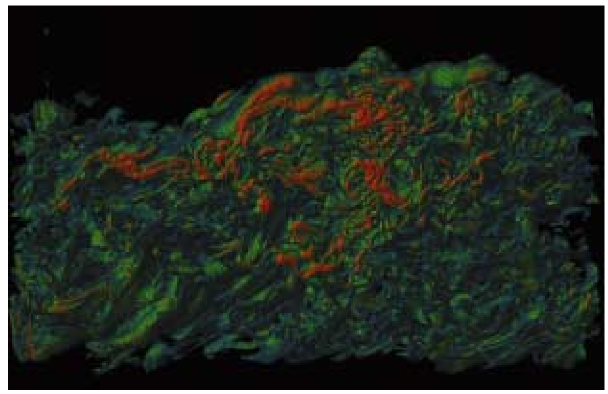


Figure 1. Viscous dissipation of the breakdown of a KH vortex caused by stratified shear flow

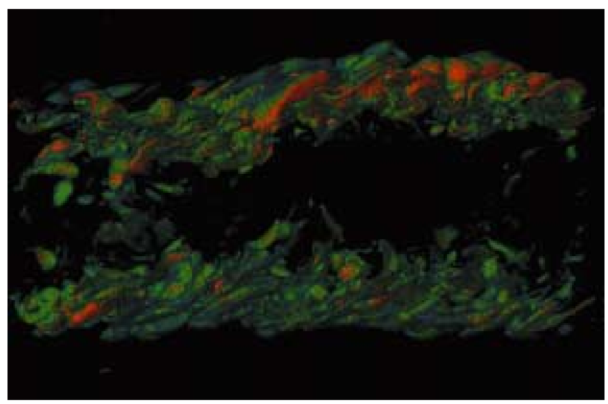


Figure 2. Thermal dissipation of the breakdown of a KH vortex caused by stratified shear flow

Figure 3. Large-eddy simulation of a swirling flow in a combustor showing the vortex flame interaction

HPCMO Benchmark

Drs. Dan Duffy, Mark Fahey, and William A. Ward, Jr.

The High Performance Computing Modernization Office (HPCMO), which guides the activities of HPCMP, organized the Benchmark Working Group to oversee the construction of a DoD HPC benchmark. This benchmark test package (BTP), as currently formulated, has three components: synthetic tests, dedicated application tests, and throughput application tests.

Synthetic benchmarks are programs that measure the performance of a computer system without doing any useful work. This is similar in concept to the way that a person's heart function is measured on a treadmill; energy is expended, cardiac performance is evaluated, but the patient does not go anywhere. Constructed by Instrumental, Inc., the synthetic tests in this BTP measure peak CPU, memory, and input/output capabilities of candidate systems.

If synthetic benchmarks correspond to a treadmill test, then application benchmarks are like walking to the store to bring home the groceries; a meaningful task is accomplished. The Computational Migration Group (CMG) at the ERDC MSRC has assembled these tests in the BTP. Thirteen actual application codes were selected for inclusion in the BTP based on MSRC utilization data. They are CHARGE, COBALT-60, CTH, FEMD, FEMWATER123, GAMESS, ICEPIC, LESlie3D, MD_MULTISCALE, NLOM, PRONTO, SARA-3D, and UNCLE. These codes represent seven of the ten computational technology areas and 70 percent of all node hours consumed at the DoD MSRCs. Four of the codes, COBALT-60 (a fluid dynamics code), CTH (a structural mechanics code), GAMESS (a chemistry and materials code), and NLOM (a weather and ocean modeling code), alone account for an estimated 32 percent of the more than 18 million node hours accrued at the four DoD MSRCs during FY 2000. These data strongly support the representativeness of this benchmarking activity.

Application codes are used in two types of tests within the BTP. The dedicated application tests involve running the codes for various inputs and numbers of processors on an otherwise empty machine in order to determine what the best possible code performance might be. The throughput application tests involve running a mix of the codes for several hours in order to gauge the system's performance in an operational sense.

The benchmark test package was copied onto CDs and made available to vendors in November 2000. Hardware vendors received copies of the test package and returned their initial results to the HPCMO on January 22, 2001. These results are currently being used by the HPCMO to provide guidance for future system procurements. The HPCMO also views production of this BTP as an initial step in a long-term performance metrics effort within the DOD HPC community.

Argonne National Laboratory

On January 9, 2000, Dr. Terry Disz, Ms. Lisa Childers, and Mr. Robert Olson from Argonne National Laboratory (ANL) and Mr. Tony Rimovsky from the National Center for Supercomputing Applications visited the ERDC MSRC to brief and exchange information with the MSRC personnel on the Access Grid multimedia conferencing system. This system, which was designed by ANL, provides multigroup collaboration across the Internet. The ERDC MSRC is installing this system and will use it to provide collaboration with users located throughout the DoD and university community.

Dr. Terry Disz, Argonne National Laboratory, briefs ERDC MSRC personnel on Access Grid

Leading-Edge Research

A partnership of Government, academic, and industry collaborators, namely, the ERDC MSRC, the Arctic Region Supercomputing Center at the University of Alaska Fairbanks, SGI, and CSC, to test an advanced supercomputing system is ongoing. The project was initiated with the installation of the Origin 3800 at ERDC. A partnership like this enhances information exchange opportunities and offers scientists the computational capability necessary to conduct leading-edge research.

Mississippi chaps Stephen Jones and Brad Comes visit Alaska in September 2000

Virginia Bedford, Technical Services Director, and Kurt Carlson, Systems Analyst, both from the Arctic Region Supercomputing Center, are shown in front of the Origin 3800 at the ERDC MSRC with Jay Cliburn, Director of System Integration and Technology, ERDC MSRC information exchange

Center of Higher Learning

On November 20, 2000, members from the Center of Higher Learning (CHL) visited the ERDC MSRC. The CHL is a consortium of three Mississippi universities and one community college located at the John C. Stennis Space Center: The University of Southern Mississippi, Mississippi State University, The University of New Orleans, and Pearl River Community College.

Members from the Center of Higher Learning are shown with Brad Comes in the ERDC MSRC scientific visualization center. Shown around table (left to right) are Dr. Adel Ali, Visualization, University of Southern Mississippi; Dr. Walt Smith, Litton; Brad Comes, ERDC MSRC Director; Dr. Conrad Johnson, University of Southern Mississippi; and Dr. Peter Ranelli, Technical Director, Center of Higher Learning

In attendance from CHL were Dr. Peter Renault, Dr. Walt Smith, Dr. Adel Ali, and Dr. Conrad Johnson. The visitors toured the supercomputing and scientific visualization centers. A possible collaborative effort between the two sites was discussed, including remote, immersive visualization.

High Performance Computing Modernization Office

The Director of the High Performance Computing Modernization Program (HPCMP), Cray Henry, along with Dr. Frank Mello, Chief Scientist, HPCMP; Dr. Larry Davis, Deputy Director, HPCMP; and John Baird, Project Manager, Shared Resource Centers, HPCMP, came to the ERDC Headquarters in Vicksburg, Mississippi, on October 31 – November 1, 2000, to visit with the ERDC Director, Dr. James Houston, some of the ERDC HPC users in the Structures and Coastal and Hydraulics laboratories, and to participate in meetings at the ERDC MSRC regarding benchmarking, system performance metrics, and Challenge Project support.

HPCMO visitors tour the ERDC Information Technology Laboratory (ITL). Pictured (left to right) John Baird, Project Manager, Shared Resource Centers, HPCMP; Brad Comes, ERDC MSRC Director; Cray Henry, HPCMP Director; Timothy Ables, ITL Acting Director; Dr. Larry Davis, Deputy Director, HPCMP; and Dr. Frank Mello, Chief Scientist, HPCMP

User Requirements—HPCMP

Tom Crimmins, Army Research Laboratory MSRC, Dr. Larry Davis, Jann Ensweiler, and Cathy McDonald, HPCMP, and Dr. Danny Weddle, Naval Air Warfare Center Aircraft Division, visited the ERDC MSRC on September 11-12, 2000, to meet with the ERDC HPC users and coordinate their requirements and HPC activities.

Dr. Robert Jensen, ERDC Coastal and Hydraulics Laboratory, discusses his HPC projects with the HPCMP team members

HPCMP team with ERDC MSRC team in the ERDC supercomputing facility. Shown (left to right) Dr. Danny Weddle, Naval Air Warfare Center Aircraft Division; Dr. Larry Davis, HPCMP; Dennis Gilman and David Stinson, ERDC MSRC; Jann Ensweiler, HPCMP; Dean Hampton, ERDC MSRC; Cathy McDonald, HPMCP; and Tom Crimmins, Army Research Laboratory MSRC

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LTG Robert B. Flowers, Commanding General, U.S. Army Corps of Engineers, January 23, 2001

CPT Jay Ferreira, ERDC; LTC Mike Kavanagh, Australian Liaison Officer, Fort Leonard Wood, Missouri; Wayne Jones, ERDC ITL; and Brad Comes, ERDC MSRC Director

MG Milton Hunter (center), Deputy Commanding General, Military Programs, U.S. Army Corps of Engineers, January 23, 2001

(Left to right) Dr. Richard Olsen, ERDC Geotechnical and Structures Laboratory (GSL); Glen Browning, ERDC MSRC; Dr. Lawson Smith, GSL; Mario Castaneda, SERNA; Paul Adams and Tom Biddlecome, ERDC MSRC; Raul Flores, GeoConsult; and Mike Valladares, U.S. Army Corps of Engineers—Tegucigalpa—Honduras, November 30, 2000

Todd Wilson, U.S. Army Engineer District, Omaha; Harry Hendler, Earth Tech Laboratory, Austin, Texas; Tyler Bowley, ERDC Environmental Laboratory; and Dennis Gilman, ERDC MSRC, December 12, 2000

U.S. Army Aviation and Missile Command representatives, Research Development and Engineering Center, Huntsville, Alabama, and David Stinson (far right), ERDC MSRC, October 25, 2000

COL James S. Weller (right front), ERDC Commander, November 7, 2000

(Left to right) COL James S. Weller, ERDC Commander; Timothy Ables, Acting Director, ERDC Information Technology Laboratory (ITL); and Deborah Dent, Special Assistant to the ITL Acting Director

(Left to right) David Stinson and MAJ Robert Sheldon, ERDC, and COL William Bailey, British Liaison Officer, Fort Leonard Wood, Missouri, September 6, 2000

The ERDC MSRC welcomes comments and suggestions regarding *The Resource* and invites article submissions. Please send submissions to the following e-mail address:

info-hpc@wes.hpc.mil

ERDC MSRC Technical Reports

00-31 "Effect of the Wave Propagation Scheme on Nearshore Wave Predictions," Stephen Wornom, David J.S. Welsh, and Keith W. Bedford.

00-32 "Practical Experiences with the Fortran Pthreads API," Clay P. Breshears and Phu Luong.

00-33 "Comparison of OpenMP and Pthreads within a Coastal Ocean Circulation Model Code," Clay P. Breshears, and Phu Luong.

00-34 "Tools for Understanding Program Performance," John Mellor-Crummey.

00-35 "Using OpenMP and Threaded Libraries to Parallelize Scientific Applications," Daniel Duffy.

00-36 "Analysis of HPC Usage: ERDC MSRC," Daniel Duffy.

00-37 "On Coupling the SWAN and WAM Wave Models for Accurate NearshoreWave Predictions," Stephen Wornom, David Welsh, and Keith Bedford.

00-38 "Effect of the Wave Propagation Scheme on SWAN Nearshore Wave Predictions," Stephen Wornom, David Welsh, and Keith Bedford.

01-01 "Emulating Co-Array Fortran with Pthreads," Richard Hanson and Stephen Wornom.

01-02 "2000 ERDC MSRC PET Training Activities," Wayne Mastin.

01-03 "PET Core Support and Focused Efforts for the period 27 March 2001 through 30 September 2001."

01-04 "FORTRAN 77 to FORTRAN 90 Source Code Conversion and Maintenance Tools," Richard Weed.

These and other technical reports can be accessed at
www.wes.hpc.mil

acronyms

Below is a list of acronyms commonly used among the DoD HPC community. You will find these acronyms throughout the articles in this newsletter.

ADPC	Automated Data Processing Center
AFOSR	Air Force Office of Scientific Research
AFRL	Air Force Research Laboratory
AFSC	Air Force Systems Command
ANL	Argonne National Laboratory
ASC	Aeronautical Systems Center
BTP	Benchmark Test Package
CFD	Computational Fluid Dynamics
CHL	Center of Higher Learning
CHSSI	Common High Performance Computing Software Support Initiative
CMG	Computational Migration Group
COE	Corps of Engineers
CPUs	Central Processor Units
CSC	Computer Sciences Corporation
CSM	Computational Structural Mechanics
CWO	Climate, Weather, and Ocean Modeling and Simulation
DNS	Domain Name System
DoD	Department of Defense
DoE	Department of Energy
DOT&E	Director of Operational Test and Evaluation
EQM	Environmental Quality Modeling and Simulation
ERDC	Engineer Research and Development Center
FDDI	Fiber Distributed Data Interface
FFT	Fast Fourier Transform
HBCU/MI	Historically Black Universities and Colleges/Minority Institutions
HPC	High-Performance Computing
HPCMO	High Performance Computing Modernization Office
HPCMP	High Performance Computing Modernization Program
IMN	Internal Major Shared Resource Center Network
ITL	Information Technology Laboratory
LFT&E	Live Fire Test and Evaluation
MCWG	Metacomputing Working Group
MPI	Message-Passing Interface
MSF	Mass Storage Facility
MSRC	Major Shared Resource Center
NASA	National Aeronautics and Space Administration
NAVO	Naval Oceanographic Office
PET	Programming Environment and Training
POM	Princeton Ocean Model
SCSL	SGI Scientific Library
SMP	Symmetric Multiprocessor
SVC	Scientific Visualization Center
TCP/IP	Transport Control Protocol/Internet Protocol
WES	Waterways Experiment Station
WMD	Weapons of Mass Destruction

training

Training Schedule*

June 5-7
HLA Regional Training Event (DMSO)

July
Computing Portals and the Grid Computing Environment (FSU)

July 31-August 2
Advanced MPI Tips and Tricks (Tennessee)

September 11-12
Advanced UNIX (OSC)

*Additional courses may be offered. Please check the ERDC MSRC Web page at ***www.wes.hpc.mil***

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Design and layout provided by the Visual Production Center, Information Technology Laboratory, U.S. Army Engineer Research and Development Center.

ERDC Major Shared Resource Center

ERDC MSRC

In Touch with Tomorrow