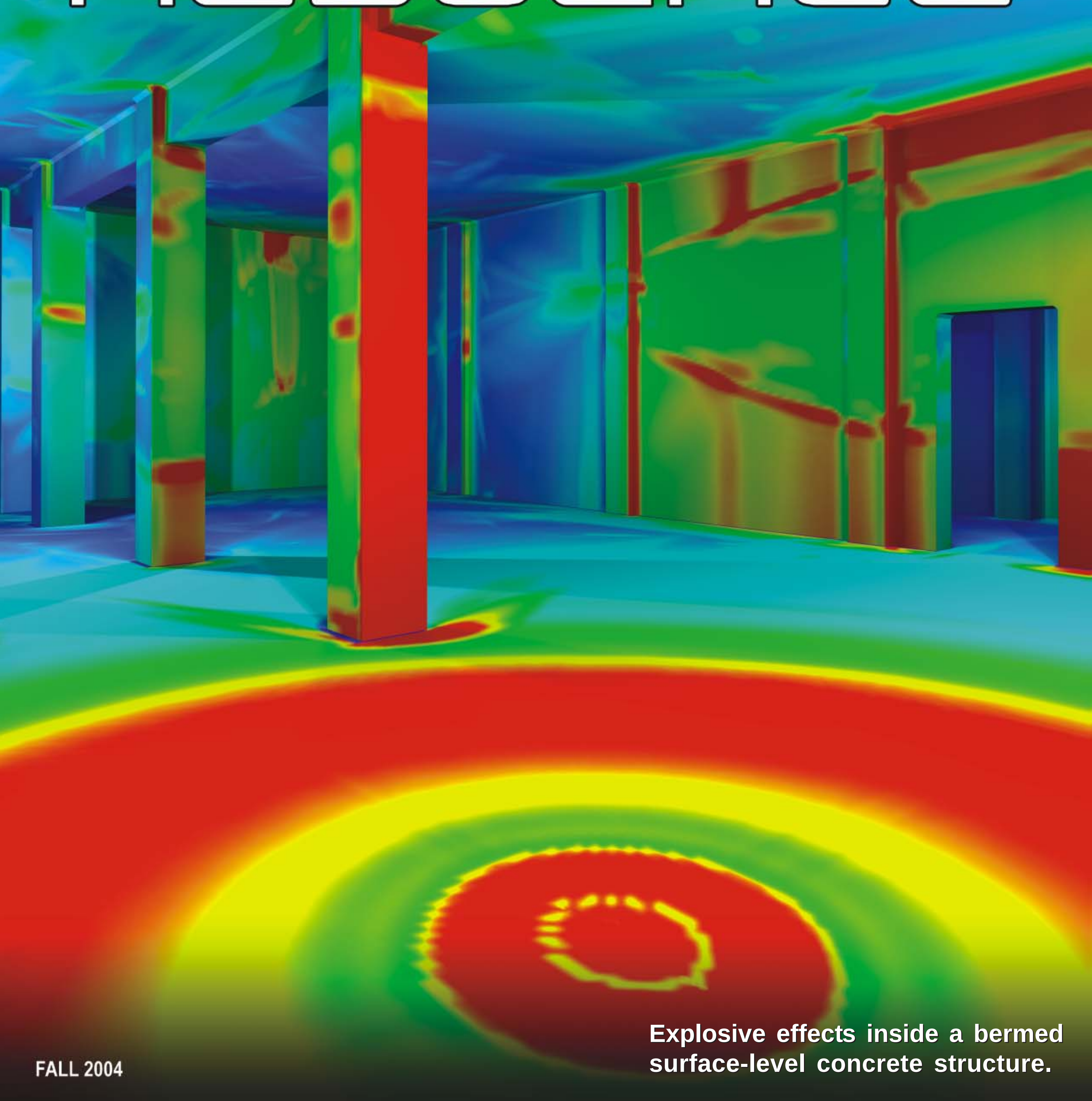
ERDC MSRC

Major Shared Resource Center

RESOURCE



Explosive effects inside a bermed surface-level concrete structure.

FALL 2004

from the director...

As I was reading through the galley proofs of this edition of the *Resource*, I was struck by how much every edition of this newsletter looks in many directions at once.

First and foremost, the *Resource* provides the vital information, tips, and techniques that you need to get your job done more efficiently and effectively using the resources of the Engineer Research and Development Center Major Shared Resource Center (ERDC MSRC). In that respect, every newsletter is very much about giving you information you can use in the here and now.

But behind the articles that focus on the here and now, there is another part of the *Resource* that looks to the future, focusing on how we are bringing the enormous talent of the ERDC MSRC to bear on the most important problems you will face as we move forward together in the years ahead.

This edition is no different. Inside its covers you'll find articles that focus on tools you can use now, like the parallel particle-tracking and code-parallelization libraries developed by our in-house computational engineering staff and the work that the queue policy working group is doing to make sure your jobs run as fast as possible. You'll also find articles that focus on both now and the future, such as those on our recent network and facility infrastructure upgrades that will ensure you will have uninterrupted access to the best computational resources the world has to offer. Rounding off this issue, as with every issue, are the articles that focus on the work we are doing together to lay the foundation for science, engineering, and technology in this country, such as our student programs and the exciting work we are doing to bring solutionHPC to reality.

I hope you are as excited by what we are doing – and what we will be doing together in the future – as I am. Our biggest task is to balance the future against the present: we have to prepare for tomorrow while ensuring that the DoD can accomplish its mission today. If you'd like to let me know how you think we're doing, drop me a line at *john.e.west@erdc.usace.army.mil*; I'd love to hear from you.

John West
Director ERDC MSRC

Front Cover:
A high performance computing SHAMRC (Second-Order Hydrodynamic Automatic Mesh Refinement Code) simulation showing MK-84 weapon delivered to a bermed surface-level concrete structure.
Back Cover:
solutionHPC – Making high performance computing easy for even the novice user. (See article, page 6).
Cover designs by the ERDC MSRC Scientific Visualization Center.

Contents

Parallelization of the WASH123D Code—Phase II: Coupled Two-Dimensional Overland and Three-Dimensional Subsurface Flows

By Dr. Ruth Cheng and Bobby Hunter

Supported by the Department of Defense (DoD) Common High Performance Computing Software Support Initiative (CHSSI) project, the parallel WASH123D code is designed to solve watershed problems on parallel scalable computers. The watershed model can solve one aspect of battlespace characterization of the environment, which includes space, weather, ocean, and soil. DoD sponsors the development of advanced technologies to develop a complete coupled battlespace environment.

WASH123D is modeled as a watershed system involving a coupled system of one-dimensional (1-D) channel network, 2-D overland regime, and 3-D subsurface media. Two environmental issues—water quantity and water quality—are addressed in this model. Two tasks, which are numerical algorithm development and code parallelization, are included in this project to improve the performance of large problem simulations.

Mathematically, 1-D channel flow and 2-D overland flow are described with the St. Venant equations, which are solved with either the semi-Lagrangian or the Eulerian finite element method. The 3-D subsurface flow is governed by the modified Richards equations, which is solved with the Eulerian finite element method.

Numerically, a parallel in-element particle-tracking algorithm for unsteady flow is employed to backtrack fictitious particles at vertices to determine the so-called Lagrangian values when the semi-Lagrangian method is used. The PT software[1] is interfaced with the parallel WASH123D code as the tool to perform the particle-tracking applications. DBuilder[2] is the software tool developed to provide a parallel programming environment.

In WASH123D, different numerical approaches are implemented to solve different components of the coupled system. The parallelization of such a complex model starts with the data structure design and then tackles the programming paradigm. The serial version of the WASH123D code is written in FORTRAN 77. Since C has better software engineering features than FORTRAN 77 and excellent library support, C is the language used to develop the parallel WASH123D. The computational kernel has no parallelization involved, and it is reused in the parallel version without any modification. Therefore, the data structure design becomes very important when the goals of object orientation, parallelization, software integration, and language interoperability need to be reached.

To account for problem domains that may include 1-D river/stream network, 2-D overland regime, and 3-D subsurface media, three `WashMesh` objects are constructed in the object `WashDomain`, which holds the computational domain as sketched in Figure 1. These three objects describe the three subdomains, on which a set of governing equations is derived to mathematically describe the behavior of the component with the entire domain. Note that the `WashDomain` also includes a coupling object named `WashCouple`. The `WashGlobal` object describes the common phenomena, and the `WashProcinfo` object sets up the parallel environment context. Each subdomain (i.e., `WashMesh`) is partitioned, based on its preferred partitioning criteria, to processors by the DBuilder. Hence, each `WashMesh` object may include `vtxDomain` and `elementDomain`, which are created and managed by DBuilder, to maintain coherent data structures among processors via ghost vertices/elements on a given mesh. The `WashCouple` may include the coupler for (1-D, 2-D), (1-D, 3-D), and/or (2-D, 3-D) interactions. The coupler encapsulates all of the implementation of a Message Passing Interface (MPI) scheme for communication/synchronization between different `WashMesh` objects. This approach can partition each subdomain (i.e., `WashMesh`) independently. Therefore, this software tool can be

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[1] J.-R. C. Cheng and P. Plassmann, “A Parallel Particle Tracking Framework for Applications in Scientific Computing,” *Journal of Supercomputing,* 28(2): 149-164, May 2004.

[2] R. M. Hunter and J.-R. Cheng, “ERDC MSRC Computational Science and Engineering (CS&E) Group Creates a New Tool for Users,” *The Resource*, pp. 6-9, Spring 2004.

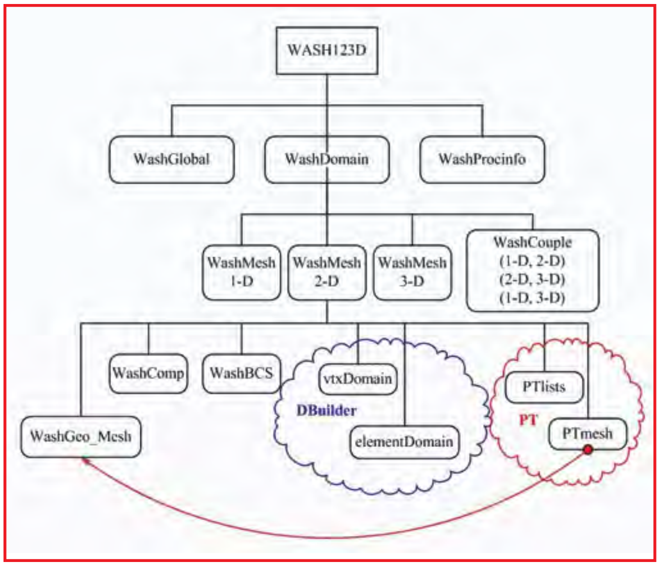


Figure 1. Data Structure Design of the parallel WASH123D

reused to integrate two or more applications with different physics on multidomains.

The nonlinear 2-D overland flow system can be linearized with the use of the Picard method. The linearized equation can then be solved by using the particle tracking to compute the total derivative term and by integrating the source/sink terms along the tracking path. Naturally, this application is perfectly suited for parallel implementation because the dependent variable, either water depth or water stage, can be obtained by solving the linearized equation independently. For such a purpose, the PT software is facilitated with a new pathline computation kernel to accurately track particles under unsteady flow fields.[3] The design goal of the PT software development is to interface with different software tools such as Scalable Unstructured Mesh Algorithms and Applications (SUMAA3d)[4] and different application codes (e.g., FEMWATER and WASH123D). This goal is achieved through a software architecture specifying a lightweight functional interface as shown in Figure 2. To efficiently incorporate different mesh (structured or unstructured) programming environments, the PT software uses an abstract particle-mesh interface (PMI), shown in Figure 2, to interact with the parallel mesh programming environment.

[3] J.-R. C. Cheng and P. E. Plassmann, "Development of Parallel Particle Tracking Algorithms in Large-scale Unsteady Flows," SIAM Conference on Parallel Processing for Scientific Computing, San Francisco, CA, Feb. 25-27, 2004.

[4] Lori Freitag, Mark Jones, Carl Ollivier-Gooch, and Paul Plassmann, "SUMAA3d Web page," *http://www.mcs.anl.gov/sumaa3d*, Mathematics and Computer Science Divison, Argonne National Laboratory, 1997.

An application is simulated for the purpose of verification and preliminary performance measurement. The conceptualized area covers about 726 square miles. To compute water flow in a watershed system, the hydro-geologic information, the topographic data, the initial conditions, the boundary conditions, and the sources/sinks must be correctly assigned to the computational mesh so that the computed flow result will reflect real flow in practice. The simulation domain consists of 2,888 vertices and 5,614 elements on the 2-D overland mesh, and 46,208 vertices and 84,210 elements on the 3-D subsurface media (Figure 3). The performance measurement is obtained on the Compaq SC45 at the ERDC MSRC. From Table 1, one can observe that the parallel efficiency is perfect at the four-way simulation and then drops to less than 50 percent at the 16-way simulation. Figure 4 shows that the communication time dominates the total time, even longer than projected ideal time, because the problem is too small to run on 16 processors. To further investigate the detailed wall clock time in communication, Table 2 lists the total number of requests and actual time

Table 1. Performance Measurement

No.of Processors (NP)	Total of Communication Time (sec)	Total Wall Clock Time (sec)	Parallel Efficiency
2	509	1,9304.1	
4	917.64	9,530.66	1.01
8	1,778.18	7,331.57	0.66
16	2,618.07	5,714.42	0.42

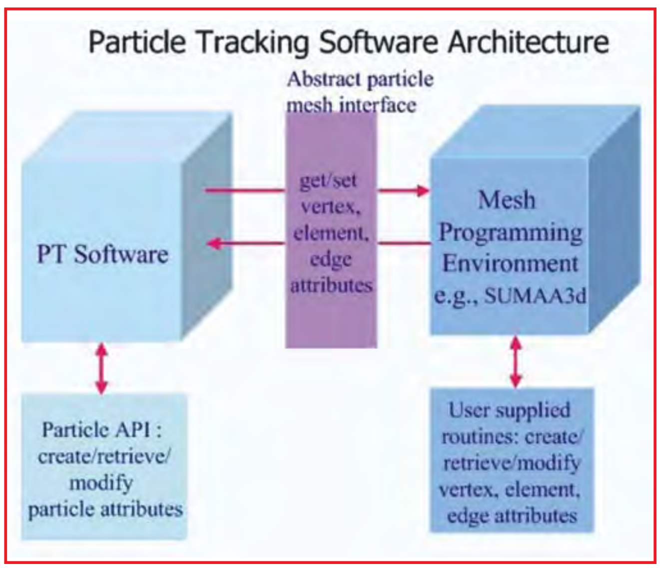


Figure 2. The particle-tracking software architecture and its interface to an existing mesh programming environment

spending in communication on different objects with respect to different physical domains. Clearly, the number of requests stays nearly constant no matter how many processors execute the simulation, but the wall clock time increases with the number of processors. Moreover, the communication time spent in the linear solver outnumbers all others, and that spent in the coupler between 2- and 3-D domain can be regarded as minor.

In summary, this phase of the CHSSI project has completed the coupled 2-D overland and 3-D subsurface system. Performance is expected to scale well for large problems. The developed tool (DBuilder) and the upgrade tool (PT) are ready for DoD HPC users to shorten their code parallelization development. In the coming year, tasks involving the 1-D channel routing and canal structure operations are to be complete.

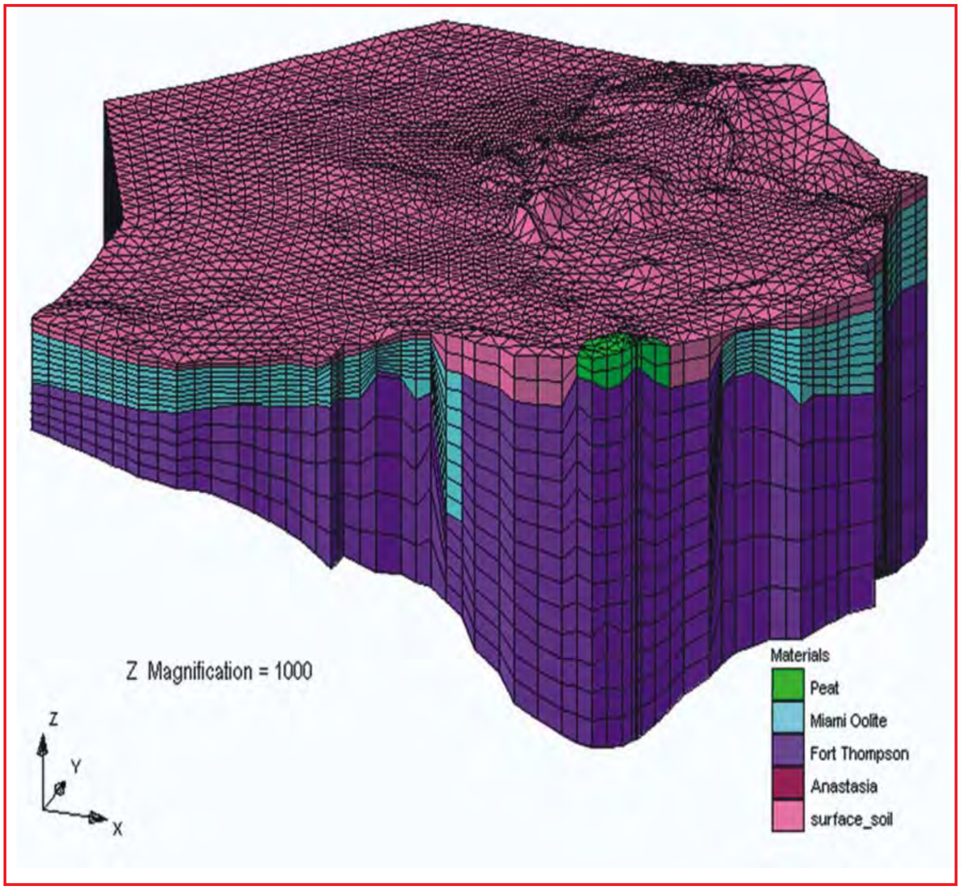


Figure 3. 2-D overland and 3-D subsurface mesh for the application

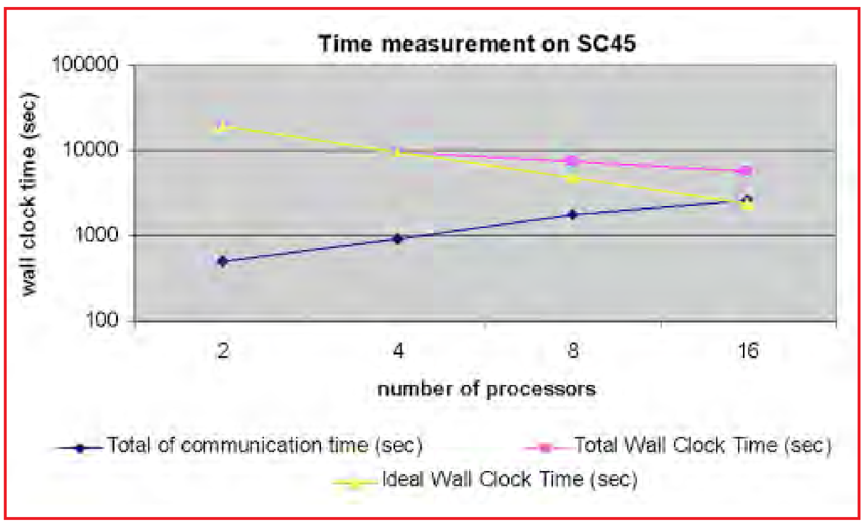


Figure 4. Time measurement on Compaq SC45

Table 2. List of Communication Time in Different Domains

NP	3-D vtxDomain		3-D elementDomain		3-D bdyDomain		2-D vtxDomain		2-D elementDomain		Coupler Update		Coupler attach	
	NC[1]	T[1]	NC	T	NC	T	NC	T	NC	T	NC	T	NC	T
2	2,647,799	488.38	3	0.0008	2,161	0.14	314,472	19.13	2	0.0001	3,245	1.36	1,081	0.04
4	2,649,200	876.86	3	0.0024	2,161	0.31	314,472	39.74	2	0.001	3,245	0.72	1,081	0.11
8	2,647,606	1,665.5	3	0.019	2,161	0.77	314,472	110.6	2	0.0056	3,245	1.28	1,081	0.31
16	2,644,916	2,385.2	3	0.0124	2,161	1.59	314,527	229.1	2	0.0014	3,245	2.19	1,081	0.64

[1*] NC: number of calls; T: time (sec).

Getting Your Work Done: The Queue Policy Working Group

By Bob Alter

Bob Alter
HPC Applications Specialist
ERDC MSRC

A Queue and Purge Policy Working Group has been formed at the ERDC MSRC. The goal of this working group is to provide recommendations on changes that should be made to queue and purge policies to ensure the most efficient allocation of computer resources to user jobs. The members of this working group are the staff personnel at the ERDC MSRC who work directly with the users, administrate the HPC systems, and can provide the expertise to implement these changes to the HPC systems.

Some of the recommended policies that are under consideration or have already been adopted include the following:

- Changes to purge policies that prevent purges of users' work directory if they have a job in the queue and are utilizing less that 300 Gbytes of workspace.
- Requiring users to put a WALLTIME limit in their batch script to allow for backfilling of jobs.
- Partitioning of jobs on the Compaq SC40 and SC45 so that individual jobs would typically get unshared nodes if the users requested a CPU count that is divisible by four.
- Limiting the number of jobs that a single user can have running at one time on a machine to allow other users a more equal chance of getting their jobs running.

Results so far have shown that large jobs with the highest priority do get scheduled to run at the earliest opportunity; but with the new backfilling policy, the machine is kept as full as possible. Evidence of this can be seen in comparing user jobs on the SGIs in April and August where the total numbers of jobs were almost identical for each month, but the number of large jobs (more than 38 percent of the machine) doubled in August as compared with April, under the new enacted queue policies.

Users who have suggestions and comments for the Queue and Purge Policy Working Group can send them by email to *msrchelp@erdc.hpc.mil*.

Paula Lindsey
Integration Life-Cycle Manager
ERDC MSRC

ERDC MSRC Upgrades Facility Infrastructure to Ensure System Availability

By Paula Lindsey

As part of ongoing efforts to create an "unbreakable" center, the ERDC MSRC recently upgraded its infrastructure in two critical areas: facility power and cooling. Reliable power is crucial to the continuous availability of high performance computing assets, and in order to ensure such availability, two new battery banks (comprised of 246 dishwasher-size wet cell batteries) were installed in the MSRC powerhouse during the week of September 12th. Each battery bank provides 1,000 kilowatts of critical power through a rotary uninterruptible power supply (UPS) to the MSRC computers during the time interval between the loss of city power and the completion of diesel-generator startup.

Each new device added to the MSRC computer room floor adds to the heat load inside the facility. To accommodate new equipment additions and to ensure the continued proper cooling of existing systems, three chiller towers that provide process chilled water for cooling in the MSRC were replaced during the week of September 20th. The new chillers increase the cooling capacity from 300 tons to 375 tons. A remote monitoring system was also installed as part of the upgrade, enabling operators to be quickly alerted to changes in chilled water system status.

The ERDC MSRC is committed to improving the computational environment and experience of its users, and these modifications, while seemingly mundane when compared to higher profile additions to or expansions of large computer systems, go far to ensure that all MSRC systems remain operational in the face of environmental challenges at the host facility.

"solutionHPC" on the Way

By Scotty Swillie

Scotty Swillie
Special Projects Lead
ERDC MSRC

A rapidly growing desire abounds within the HPC community for a more comprehensive, user-friendly approach to resource access and utilization. New and less experienced users need an entry point that unlocks the power of the HPC world in a way that flattens the learning curve and leads to new discoveries. In response to this need, the ERDC MSRC is launching a new project, "solutionHPC."

Creating a project circle that users can travel as effortlessly as possible is the overall goal of solutionHPC. The key to making this a reality is by abandoning the old stovepipe model approach and taking a system approach. To do this, barriers between the three major phases of the HPC process – computation, visualization, and storage – are being broken down. This process focuses on ease of access and use as well as how each phase will integrate into a seamless workflow with the other phases. In response to a question about the scope of this project, John E. West, Director, ERDC MSRC, said, "This is a huge undertaking, but one worth tackling because of the wealth of new science that may be realized."

The central element that will tie the solutionHPC system together will be an Application Programming Interface (API). The API will reside on a secure server inside the HPC network. It will allow a high level of expandability by serving as a platform that software developers can program against. This interface will offer users of all experience levels a complete toolkit that will enable them to fully manage jobs, schedule/view visualizations, store results, and search/access past results. The solutionHPC interface will feature the look and feel of a Web site with links and visual representations of job progress and system availability. The look and feel will be intuitive to a level that allows even the novice user the ability to begin making progress quickly.

"The visual element of solutionHPC will help bring to light discovery in areas that may have been previously hidden within a researcher's code."

– **John West**
Director, ERDC MSRC

An unfortunate fact is that the overwhelming majority of HPC jobs are never visualized effectively. solutionHPC hopes to change this by focusing on the "I see" and "We see" modes of exploration. Using either a batch or interactive method, users will be allowed to select an imaging tool, schedule basic visualizations of a project, and have the images returned for viewing directly within the interface. This process will provide users with the opportunity to visually track the progress of a job at a level never before available. "The visual element of solutionHPC will help bring to light discovery in areas that may have been previously hidden within a researcher's code," John West added.

Storage of completed jobs is the final major component within the solutionHPC system. Because of the difficulty users have in retrieving information about what is in stored files, users are missing hidden nuggets of information from files that may be 5 or 10 years old that could be useful when planning new work. solutionHPC will offer a storage component that is powerful and user-friendly. File transfer/retrieval will be greatly simplified, and a database will be used to store metadata about each job. This will allow the interface to display a listing of relevant jobs by user, title, software used, or one of many other descriptors. This smart storage component of solutionHPC will complete the project circle.

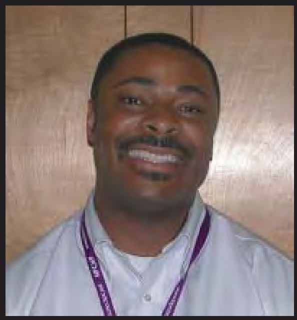
Once the individual components are complete, they will be blended into the comprehensive solutionHPC system. The finished system will offer powerful research tools with one-stop access to the world of high performance computing. The resulting ease of use and increased turnaround times will allow higher levels of research to be done in shorter time frames. This swings open wide the door of discovery and allows the users of solutionHPC to realize the full potential of their research.

Nurturing the Next Generation . . .

Attracting the best and brightest students to science and engineering remains one of the top priorities for the ERDC MSRC in its effort to help ensure technological leadership for the next generation. During the past 12 months, it has devoted 4,490 total contact hours toward this effort with 1,194 of those hours concentrating on minority students. During the summer of 2004, the ERDC MSRC participated in three major outreach efforts that will help shape the future of the science and engineering work force.

HPC Summer Institute

By Reginald Liddell



Reggie Liddell
PET Training Coordinator
ERDC MSRC

The ERDC MSRC and the High Performance Computing Modernization Program Programming Environment and Training (PET) program, in partnership with Jackson State University (JSU), held its 6th HPC Summer Institute for graduate and undergraduate students from minority serving institutions nationwide. On Monday, June 14, the Institute conducted orientation and opening sessions for 14 students representing six universities for 2 weeks of HPC learning activities.

John E. West, ERDC MSRC Director, gave a presentation to Institute participants and faculty entitled "User Perspectives on HPC and How to Prepare for Careers in Supercomputing." The lecture focused on the many uses of supercomputing in the scientific and engineering communities as well as on the open research issues in HPC and possible career paths for young researchers. Dr. Joe Thompson, Mississippi State University (MSU), and Paul Adams, ERDC MSRC Scientific Visualization Center Lead, hosted lectures on "Supercomputing in Mississippi" and "Scientific Visualization," respectively.

The Institute coordinated a tour of the ERDC MSRC research site hosted by Dr. Wayne Mastin and Reggie Liddell, both of the PET program. Dr. Deborah Dent, ERDC Information Technology Laboratory (ITL) Deputy Director, spoke with the students during lunch. She expressed the importance of academic achievement, work ethic, and the ongoing demand for top quality IT professionals in the HPC industry. Week One Institute activities concluded with a tour of the Engineering Research Center at MSU with Dr. Robert Moorehead serving as point of contact.

Program activities designed to introduce participants to the world of HPC, included (1) Building Clusters with Linux Servers, (2) Applications of Scientific Visualization, (3) Introductions to Virtual Reality, (4) High Fidelity Simulation, (5) Foundations and Applications of Computational Fluid Dynamics, and (6) Applications of Enabling Technologies. Students paired into six groups, each assigned to a mentor for project and presentation support. HPC practitioners from ERDC, JSU, MSU, and the University of Alabama, Birmingham (UAB), served as mentors for the students, who enabled them to help connect course material to real-time hands-on examples of typical HPC ventures.

Week Two learning activities and closing ceremonies concluded at UAB, Friday June 25. Many of the students showed keen interest in the possibilities and the vast array of HPC opportunities. Edward Tate, a senior computer science major at Southern University, remarked of how overwhelming and impressed he was to see the level of technology housed at ERDC. Senior computer science majors from Hampton University, Ashley Brooks and Roshawnda Walker, explained how their classmate Brittany Owens raved about her 2003 summer intern experience, which inspired them to apply for the 2004 HPC Summer Institute.

more . . .

The Institute is part of a longstanding series of Institutes held by the MSRC, PET, and JSU to expand awareness of, and interest in, science, engineering, and supercomputing among traditionally underrepresented groups. The selected engineering and computer science majors for the Institute for 2004 included six students from JSU, Jackson, MS, two students from Hampton University, Hampton, VA, one student from Mississippi Valley State University, Itta Bena, MS, one student from Alabama A&M University, Huntsville, AL, three students from Southern University-Baton Rouge, Baton Rouge, LA, and one student from Rust College, Holly Springs, MS.

JSU Institute participants are shown with ERDC MSRC personnel PET Component 3 Program Manager Dr. Wayne Mastin (far left), ERDC MSRC Director John E. West (second from left), and PET Component 3 Technical Advisor Bob Athow (far right)

Those interested in applying for the program should contact Dr. Loretta Moore by e-mail at loretta.a.moore@jsums.edu or telephone at (601) 979-2105.

S.A.M.E. Engineering and Construction Camp

By Rose J. Dykes

Thirty-nine high school juniors and seniors from Louisiana and Mississippi attended the second annual S.A.M.E. (Society of American Military Engineers) Engineering and Construction Camp held at ERDC, Vicksburg, Mississippi, during the week of June 6-12. Dr. Michael Stephens, ERDC MSRC Scientific Visualization Center (SVC) and the Army High Performance Computing Research Center, served as one of the instructors when the students visited the Information Technology Laboratory.

Dr. Stephens demonstrated an interactive computational fluid dynamics (CFD) application on the SVC's Immersadesk. He then allowed the students to drive the application where they moved around in the fluid flow and released virtual smoke streams to investigate the flow fields.

Dr. Michael Stephens, ERDC MSRC, demonstrates an interactive computational fluid dynamics virtual reality application on the Immersadesk

The purpose of this camp is to give high school students hands-on experience in engineering and construction skills in Vicksburg's wide-ranging engineering community as the students perform various curriculum activities at each of the ERDC-Vicksburg laboratories. The Vicksburg and Louisiana Posts of S.A.M.E. host the camp. Professional engineers and volunteers from local engineering organizations supervise the program.

PET Summer Intern Program

By Dr. Wayne Mastin

Dr. Wayne Mastin
PET Component 3 Program Manager
ERDC MSRC

The PET Summer Intern program completed another successful 10-week term on August 6, 2004. The group of students this summer consisted of a record number of six interns, including students from Pennsylvania, Arizona, and Hawaii.

The first few years of the PET Summer Intern program operated on a modest scale. From 1997 through 2000, Clark Atlanta University sent one student to ERDC each summer. If the intern program is judged only on the basis of contributing to the DoD work force, these first few years were a success. The last intern provided through Clark Atlanta, Richard (Rikk) Anderson, subsequently was hired at the ERDC MSRC and developed the Big Brother HPC machine monitoring system.

Beginning in the summer of 2001, students were recruited from all colleges and universities and funded directly by PET. The program is now administered by the University of Hawaii, under contract with Mississippi State University. Students are recruited from across the Nation for all four of the High Performance Computing Modernization Program (HPCMP) MSRCs. Although no preference is given to local institutions, generally about half of the interns come from Mississippi and adjoining states. Many of the recent interns are still pursuing their education. One intern from the summer of 2003, Leelinda Parker, graduated from Jackson State University and accepted a position with the Army Research Laboratory.

This summer's interns addressed a wide variety of challenging problems in collaboration with their mentors in the ERDC MSRC. Jennifer Williams, an applied mathematics major at the University of Alabama in Birmingham, worked on the analysis and visualization of HPC performance data. This work will assist her mentor, Dr. Bill Ward, and others in the Computational Science and Engineering group in the interpretation of performance characteristics of ERDC MSRC hardware and software resources.

Omar Rodriguez, computer science major at Arizona State University, returned for his second summer as an intern at ERDC. He continued working with his mentor, Dr. Wayne Mastin, on efforts supporting the PET Online Knowledge Center by developing and implementing a structure for the PET program's online training resources.

Jian-Zhong (Dan) Li, computer science major from Bucknell University, developed scripts for his mentor, Jay Cliburn, to improve the system monitoring capabilities for the MSRC's HPC machines.

Si Loi Leung, mechanical engineering major at the University of Hawaii, worked with his mentor, Nathan Prewitt, on the investigation of techniques used in automatic grid generation for complex geometric shapes.

Corey Bordelon, a computer science major at the University of Louisiana, Monroe, developed a Web-based task manager system for the Desktop Support team. Corey's work was done in collaboration with his mentor, Morris Ramsey, along with Rikk Anderson and Karen Mauldin.

The final intern for the summer of 2004 was Kylie Nash, a computer science major at Jackson State University. She worked with her mentor, Paul Adams, on several visualization projects during the 4 weeks she spent at the ERDC MSRC.

The success of the PET Summer Intern program is due not only to the interns and mentors but also to the efforts of the PET staff: of significant note are Anne Mullins, who provided administrative and logistics support, and Reggie Liddell, who organized the intern lecture series that enriched the educational experience of the interns. The students indicated their internship was a rewarding experience and expressed an interest in returning to Vicksburg next summer.

Students interested in applying for next year's program should contact Dr. Susan Brown by e-mail at stbrown@hawaii.edu or telephone at (808) 956-2808.

PET interns shown (left to right) are Corey Bordelon, Si Loi Leung, Jennifer Williams, Omar Rodriguez, and Jian-Zhong (Dan) Li

ERDC MSRC Upgrades Network

By Jay Cliburn

Prior to this upgrade, the ERDC MSRC was not behind a firewall; now it is. Occasionally, a network configuration change at the user end may result in blocked IP traffic at the MSRC firewall.

Jay Cliburn
Technical Operations Manager
ERDC MSRC

Over a 4-day period in July, the ERDC MSRC replaced its entire internal network infrastructure in order to provide redundancy, higher fault tolerance, and improved performance to local and remote users and staff. A central architectural feature of the new configuration includes dual, redundant, highly available pathways from the Defense Research and Development Network (DREN) to HPC and mass storage systems. Specific network components of interest include the following.

- Dual Netscreen 5200 firewall devices to detect and deter unauthorized intrusion, and to provide detailed network traffic logging information to assist in post-intrusion forensics. These devices also provide border router functionality for the MSRC.
- Dual high-speed Foundry BigIron 4000 core switches to provide 10 gigabit connectivity to the DREN and pass 1 gigabit traffic into the MSRC.
- Dual high-speed Foundry BigIron 15000 distribution switches to distribute 1 gigabit traffic throughout the MSRC.
- Dual 1 gigabit network interfaces for the mass storage system and most HPC system user logins, and dual gigabit data pipes between HPC systems and the mass storage archive for redundant data transfers to and from the mass storage system.
- Addition of 100/1,000 megabit per second (Mbps) capability to staff desktops and other edge devices.

The new network will be IPv6 compatible and also supports 9,000-byte Ethernet network packets, called “jumbo frames.” Typical Ethernet packets are 1,500 bytes in size; jumbo frames provide for more efficient data transfer, resulting in increased throughput, especially for large files that are common in scientific computing. The new network is also 10-gigabit ready throughout, enabling the next uptick in network speed without the need for chassis replacement of network gear and the associated lengthy downtime and user disruption accompanying that activity. (Translated, a “forklift upgrade” won’t be required to go to 10 gigE.)

Of particular interest to users (and their respective local network administration staffs) is the addition of the Netscreen firewall devices. Prior to this upgrade, the ERDC MSRC was not behind a firewall; now it is. Occasionally, a network configuration change at the user end may result in blocked IP traffic at the MSRC firewall. If you suspect this to be the case, please contact the Customer Assistance Center for help.

The ERDC MSRC is pleased to provide this improved network infrastructure to its users. The network is faster, more resilient, and more secure than ever before, and it is extensible to the next generation of LAN bandwidth, standing well to provide service to the HPCMP community for the next several years.

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

msrchelp@erdc.hpc.mil

ERDC MSRC Exhibits High Profile at Users Group Conference 2004

By Rose J. Dykes

Rose J. Dykes
Writer/Editor
ERDC MSRC

Personnel from the HPCMP computing centers and the users of these resources gathered in Williamsburg, Virginia, June 7-11, for the Users Group Conference 2004, where a forum was provided for communication, training, and discussion of HPC and its impact on science and technology. ERDC MSRC team members participated by conducting tutorials and presenting technical papers and other talks, thereby helping to ensure that the DoD community has the tools and expertise to make the best use of state-of-the-art systems.

On the first day of the Conference, Paul Adams, Tom Biddlecome, and Richard Walters, all of the ERDC MSRC Scientific Visualization Center, conducted a full-day Bring Your Own Data Workshop. Dr. William Ward and other members of the ERDC MSRC Computational Science and Engineering group along with Cray, Inc., staff conducted a full-day tutorial entitled "Cray X1 Code Migration and Optimization."

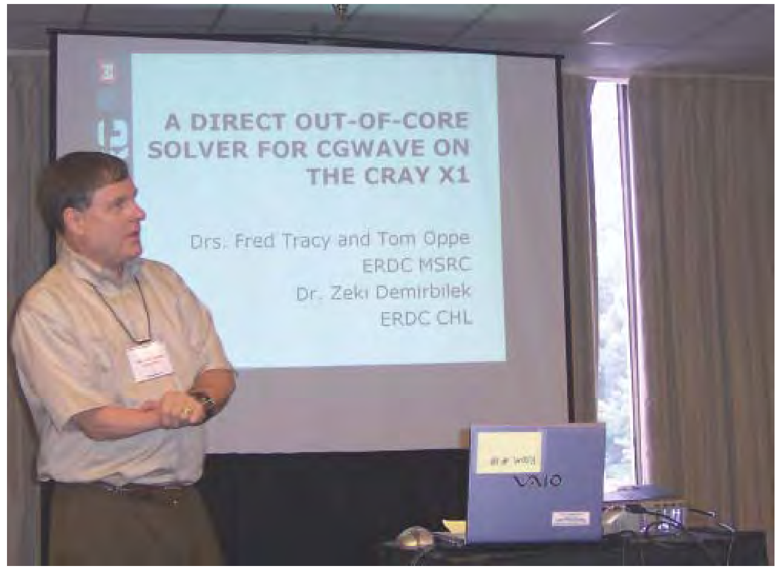
Dr. Fred Tracy presented two technical papers at the Conference, one entitled "Optimizing Finite Element Programs on the Cray X1 Using Coloring Schemes" and the other "A Direct Out-of-Core Solver for CGWAVE on the Cray X1," stressing that sizeable speedup can be achieved on the ERDC Cray X1 by modifying key algorithms and using specialized compiler directives.

Other presentations by ERDC MSRC team members were as follows: "DBuilder: A Parallel Data Management Toolkit for Scientific Applications" by Bobby Hunter; "Performance of a Synthetic Application of Benchmarking on Several High Performance Computing Platforms" by Dr. Paul Bennett; "Experiences Profiling and Characterizing DoD HPC Applications" by Dr. William Ward; "A Configuration Exploration" by Carrie Leach; "OKC: A Quick Look at the PET Online Knowledge Center" by Lesa Nelson; "RSS: Using Really Simple Syndication to Keep Users Informed" by Glen Browning; and "Memory Debugging of Parallel Programs: Issues, Tools, and Experiences" by Dr. Jeff Hensley.

A highlight at the Conference for the ERDC MSRC was having its Scientific Visualization Lead, Paul Adams, receive the HPCMP "Technical Excellence" award. This is given to the nominee who best demonstrates scientific or engineering excellence using HPCMP resources in a creative and effective manner. Paul along with his team at ERDC accomplished this by integration of scientific data with animation, as shown in the graphic below in which an isosurface of water values is rendered as realistically as possible.

Large-eddy simulation of steep breaking waves and thin spray sheets around a ship

Dr. Fred Tracy presents one of his two paper presentations at the Conference



Dr. Bob Maier (center) and Paul Adams (far right) talk about work at the ERDC MSRC with a visitor at the Conference Poster Session

Glen Browning makes his RSS NewsFeed presentation to a standing-room only crowd at the Conference

Cray User Group Conference

Dr. Sam Cable
Computational Engineer
CS&E, ERDC MSRC

Dr. Thomas Oppe
Computational Engineer
CS&E, ERDC MSRC

Drs. Sam Cable and Thomas Oppe of the Computational Science and Engineering (CS&E) group at the ERDC MSRC presented a paper entitled "Optimization of LESlie3D for the Cray X1 Architecture" at the Cray User Group conference held in Knoxville, TN, on May 17-21. LESlie3D is a Computational Fluid Dynamics (CFD) code developed at Georgia Tech that is used for solving turbulent reacting flows such as those occurring in combustion chambers. A version of this code for structured meshes was optimized for the X1 architecture by the insertion of compiler directives to increase vectorization and multistreaming efficiency. The optimized code ran approximately 20 percent faster than the original code and performed more vector operations. In addition, a comparison of the original and optimized versions of LESlie3D was made using hardware counter data obtained from the ERDC X1 and from an IBM p690 computer at the Naval Oceanographic Office (NAVO) MSRC. For a 16-processor run of LESlie3D using a grid of 192^3, the optimized code ran over 12 times faster on the X1 than on the IBM at the MSP level and three times faster on the SSP level. The code also exhibited better cache behavior on the X1 than on the IBM.

Dr. Bill Ward
CS&E Group Lead
ERDC MSRC

University of Southern Mississippi

Dr. Bill Ward, Lead for the ERDC MSRC CS&E group, visited the University of Southern Mississippi and spoke to students on the subject of research ethics. The audience included students from "Introduction to Computing" and "Computer Ethics" classes in the Computer Science (CS) Department and from a "Computer Ethics" class in the Criminal Justice Department. Dr. Ward began with some general remarks on morality, ethics, and integrity and then discussed several case studies related to ethics in research. Ms. Nancy Howell, the instructor for the CS ethics class described the presentation as "on target" and said she hoped to repeat the presentation during the fall semester.

Mississippi Governor Haley Barbour Visits ERDC

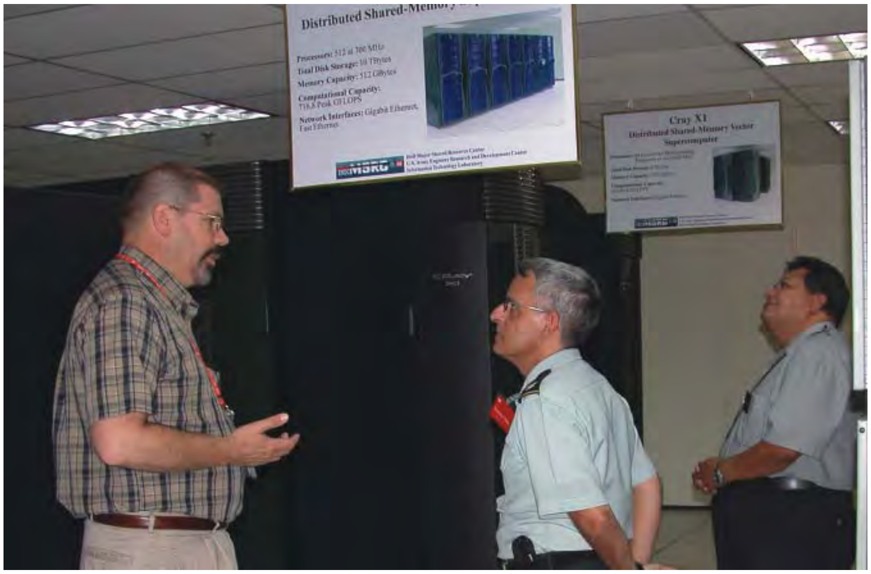
Governor Haley Barbour visited ERDC on August 6, 2004. The Governor, who took office earlier this year, is visiting government agencies and industry around the state of Mississippi to familiarize himself with their missions and capabilities. A briefing on the organization's mission to support the warfighter and the civil works activities of the Corps of Engineers was presented to him before he toured each of the ERDC's four Vicksburg laboratories.

Governor Barbour arrives at the ERDC Information Technology Laboratory

At the ERDC MSRC, Governor Barbour toured the HPC center viewing the computing resources and learning about its computing capability. The MSRC's state-of-the-art techniques for data interpretation were also discussed. In addition, the Governor was made aware that the MSRC realizes the importance of attracting the best and brightest students to science and engineering and, therefore, continually participates in programs that promote this.

Dr. Jeffery Holland (far right), ERDC Information Technology Laboratory Director, talks with Mississippi Governor Haley Barbour and others during the Governor's visit to the MSRC, August 6, 2004

Information Technology Laboratory Director Dr. Jeffery Holland discusses a scientific visualization project with Governor Barbour



(Left to right) David Stinson, ERDC MSRC Assistant Director, with COL Manuel Fuentes, Inspector General, Joint Force Headquarters, Mississippi Army National Guard, and Miguel Gonzalez, U.S. Army Engineer District, Vicksburg, Vidalia, LA, Area Office, September 15, 2004

(Left to right) COL Todd Semonite, Office, Chief of Engineers, The Pentagon, Dr. Bob Maier, ERDC MSRC Assistant Director, and COL Jim Rowan, ERDC Commander, June 4, 2004

Greg Rottman (far left), ERDC MSRC Assistant Director, with U.S. Army Engineer Division, South Atlantic, Emerging Leaders, May 12, 2004

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.

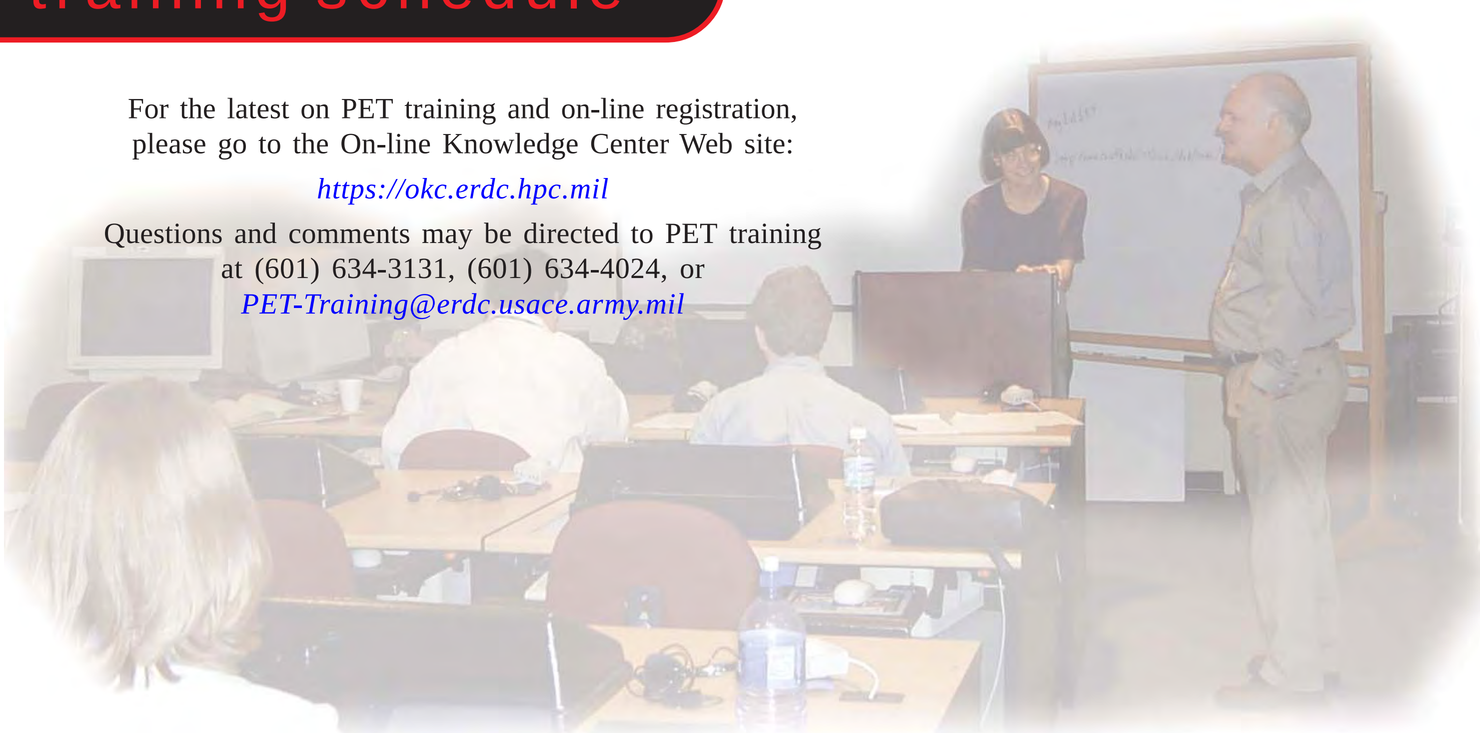
API	Application Programming Interface
CFD	Computational Fluid Dynamics
CPU	Central Processing Unit
CS	Computer Science
CS&E	Computational Science and Engineering
DoD	Department of Defense
DREN	Defense Research and Development Network
ERDC	Engineer Research and Development Center
HPC	High Performance Computing
HPCMP	HPC Modernization Program
ITL	Information Technology Laboratory
JSU	Jackson State University
MPI	Message Passing Interface
MSP	Multistreaming Processor
MSRC	Major Shared Resource Center
MSU	Mississippi State University
NAVO	Naval Oceanographic Office
PET	Programming Environment and Training
PMI	Particle-Mesh Interface
PT	Particle Tracking
SHAMRC	Second-Order Hydrodynamic Automatic Mesh Refinement Code
SSP	Single-Streaming Processor
SVC	Scientific Visualization Center
UAB	University of Alabama, Birmingham

training schedule

For the latest on PET training and on-line registration, please go to the On-line Knowledge Center Web site:

https://okc.erdc.hpc.mil

Questions and comments may be directed to PET training at (601) 634-3131, (601) 634-4024, or *PET-Training@erdc.usace.army.mil*



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For more, see page 6.

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