

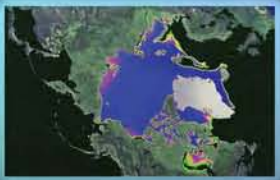
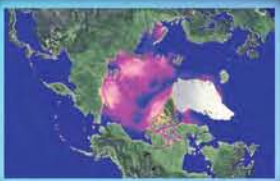
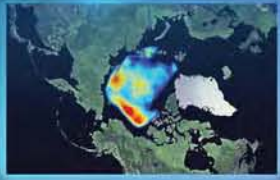
NEWSLETTER

*The*

SPRING 2004

# Resource

U.S. ARMY ENGINEER RESEARCH AND DEVELOPMENT CENTER  
INFORMATION TECHNOLOGY LABORATORY



Major Shared Resource Center

# ERDC IVISR



**HRC**  
Modernization Program

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## *From the Director*

As I write this article, two things come to mind that I want to communicate to our newsletter recipients. The first is the goal of the U.S. Army Engineer and Research and Development Center (ERDC) Major Shared Resource Center (MSRC) (through the Department of Defense (DoD) High Performance Computing Modernization Program (HPCMP)), which is to deliver high performance computing (HPC) leadership, service, education, and technical expertise to achieve research and engineering objectives vital to the Nation.

Helping to provide the U.S. warfighter the advantage on the battlefield by means of HPC is of utmost importance to this Center. The largest impact that our Center can have to accomplish this is by providing our users the latest in HPC and by striving to make the effective use of these resources easier.

The second thing is recognizing the importance of helping to shape the future with outreach efforts in educational institutions to boost science and engineering, thereby helping to enable the United States to regain leadership in technology. According to Warren Washington, Chairman of the National Science Board, which oversees the Federal National Science Foundation, our country is in a race to retain its global advantage in science and engineering.

Much of the information that we have chosen to publish in this edition of our newsletter supports my thoughts above. Day-to-day challenges that our Program faces must not overshadow our purpose here at the ERDC MSRC. With our dedicated staff, we will continue striving to provide our users with the latest technology and the help through training and innovative solutions by our staff to use it. We will continue with our outreach effort to attract the best and brightest students to science and engineering and retain them to ensure technological leadership for the next generation.

John West  
Director, ERDC MSRC

### **About the Cover:**

Front Cover: Using high performance computing in the modeling of ocean water containing sea ice (see article, page 2).

Back Cover: RSS Newsfeed (see article, page 26).

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# HPC at Work . . . . .

## *Ocean Modeling Using High Performance Computing*

By Dr. Fred T. Tracy and Tommy L. Biddlecome, ERDC MSRC, ITL, and Dr. Wieslaw Maslowski, Department of Oceanography, Naval Postgraduate School

The ability to predict narrow (of order 10 km) and long (of order 1,000 km) features in sea ice is of great interest and importance to the U.S. Navy submarine fleet operations in the region. A team of researchers from the Naval Postgraduate School (NPS) in Monterey, California, led by Dr. Wieslaw Maslowski, has been involved in the development of the Polar Ice Prediction System (PIPS) 3.0 test model. This is a part of an effort sponsored by the Office of Naval Research to upgrade the Navy operational PIPS model. The final setup for ice/ocean modeling is still under development. The main emphasis of the research discussed in this article is on improvements of the modeled sea ice, leading to better prediction of open-water regions within the ice pack or so-called leads and polynyas frequently observed in the Arctic Ocean.

One of the requirements to advance model skill in predicting leads and polynyas involves increasing model horizontal (and vertical) grid-cell resolution. In the PIPS 3.0, model resolution is increased to 1/12-degree (or ~ 9 km) and 45 vertical levels from

17 to 33 km and 15 levels in PIPS 2.0 (see Preller et al. 2002, for more details). The test grid uses the rotated coordinate system to eliminate a singularity problem at the North Pole and to minimize the latitudinal grid convergence. The test model domain (Figure 1) includes the North Pacific (from about 30N), the proper Arctic Ocean with the Canadian Archipelago and the Nordic Seas, and the North Atlantic (to about 45N). This approach allows the test model to account for all the northern latitude ice-covered regions at a high and nearly uniform resolution.

Another, more logistical requirement is related to a specific architecture target for running the PIPS 3.0 test model. The U.S. Navy Fleet Numerical Meteorology and Oceanography Center (FNMOC) has committed to the modern SGI multiprocessor technology, such as the Origin 2000 (O2K) and 3000 (O3K) machines in their recent operational system upgrades. This fact imposed an immediate demand for changing the existing NPS ocean and sea-ice model codes (Maslowski et al. 2000, Maslowski et al. 2001) from using SHMEM on Cray

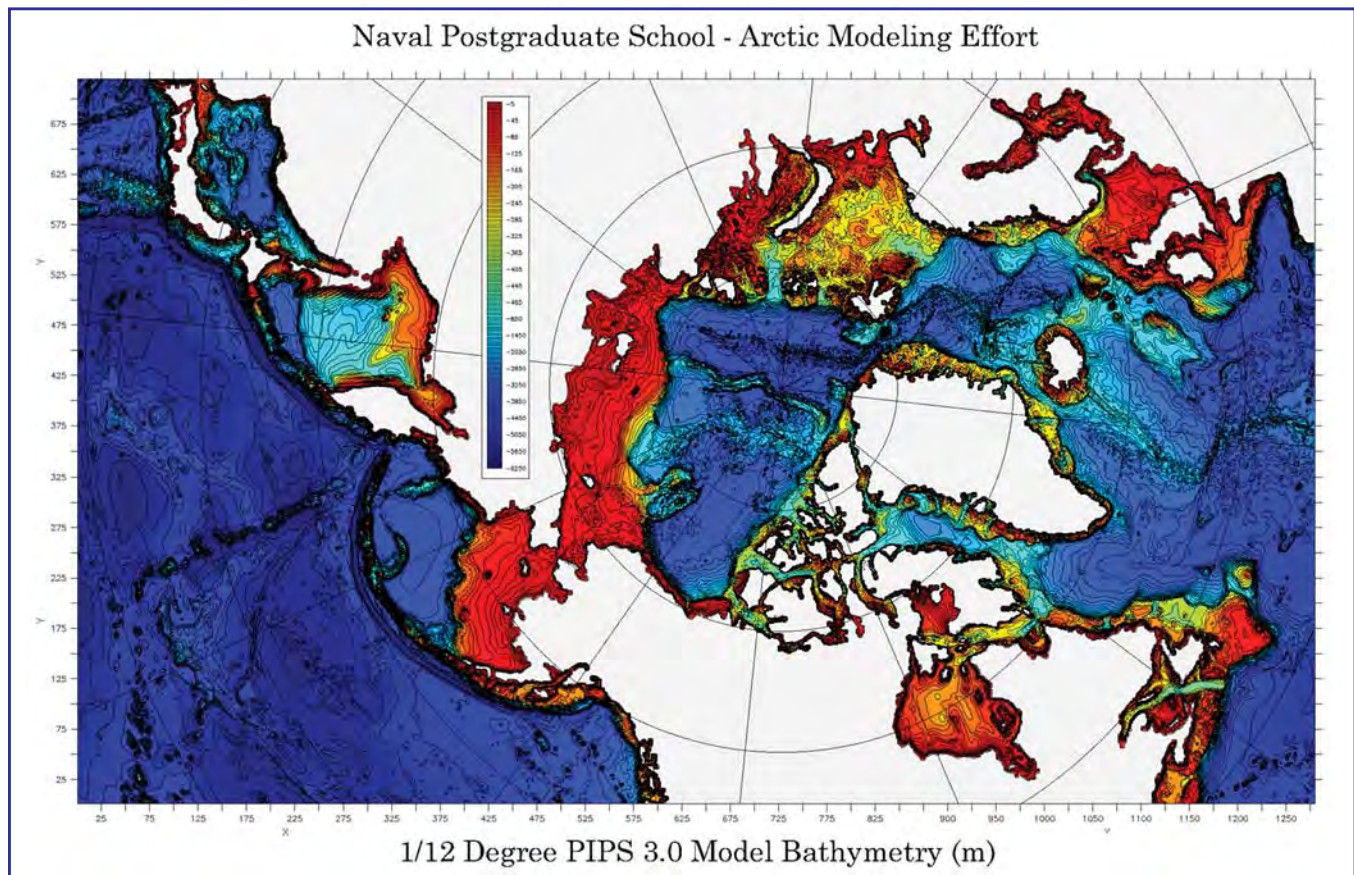


Figure 1. Test model domain

T3E machines to the Message Passing Interface (MPI) on the SGI computers. In addition, timely information about the performance of the MPI version of the PIPS 3.0 test code on the O3K at ERDC was critical to determine resources needed for the PIPS 3.0 on the O3K computer dedicated to run the Navy operational codes at FNMOC.

Support of Dr. Maslowski began with Dr. Mark Fahey, ERDC MSRC Computational Science and Engineering (CS&E) group (now at Oak Ridge National Laboratory, Oak Ridge, Tennessee). Dr. Fred Tracy, CS&E group, and Dr. Fahey ported the T3E SHMEM version of PIPS 3.0 to the SGI O3K. SHMEM works on the O3K, but adherence to the rule that data objects being sent and received must be symmetric or remotely accessible is critical. A symmetric array or variable has the same size, type, and relative address on all processing elements (PEs). One can consider the one-sided 64-bit get shown below.

```
call shmem_get64 (y, x, n, ipe)
```

where n pieces of 64-bit data are moved from x to y. Tracing variables such as x and y back through the levels (sometimes several subroutines) of the various calls was done to ensure that when they were originally defined, they were in a common block rather than a dimension statement. Variables in a common block are symmetric, whereas variables defined by dimension statements are not. With a liberal use of barriers for synchronization, the SHMEM version then worked.

A joint effort between Drs. Maslowski and Tracy has resulted in a new MPI-based coupled test ice-ocean model. To do this quickly, a set of four MPI routines were written using standard MPI (Version 1.1) calls that reproduced the capability of the one-sided communication SHMEM gets and puts. One-sided communication is written in the MPI-2 standard but was not implemented on many architectures at that time. This approach took far less time than a complete rewrite of the message-passing part of the PIPS 3.0 test code. This new code has been evaluated on the ERDC O3K complex using resources of the NPS Challenge Project. Table 1 shows a comparison of PIPS 3.0 performance using the SHMEM version and the new MPI version

<b>Communication</b>	<b>Number of PEs</b>	<b>Time (sec)</b>
SHMEM	32	1,484.71
MPI	32	1,708.34
SHMEM	64	991.92
MPI	64	1,054.85

for a test data set on the ERDC O3K complex using 32 and 64 PEs. For a short-term effort, the results are good.

The test model results show a dramatic improvement in the modeling of sea ice and ocean behavior in response to the prescribed atmospheric forcing. One of the most challenging aspects of modeling the Arctic sea ice is to properly represent its thickness distribution throughout the basin. In Figure 2, the 3-year mean sea-ice thickness distribution for 1979-81 is presented. The modeled distribution of ice thickness compares reasonably well with that known from observations. Many regions are located in the Arctic Ocean where the sea-ice and ocean observations are limited. In that respect, model results are potentially useful in not only forecasting ice thickness and ice-edge variability but also in guiding future field campaigns to better understand environmental changes in this region.

Case-specific scientific visualization techniques were developed by the ERDC Scientific Visualization Center (SVC) staff for both model verification and data exploration (Fang et al. 1998) using Dr. Maslowski's ocean data. Figures 3 and 4 show example results of this work. Within the domain of large data sets such as this test model, unique difficulties exist in exploration and evaluation. Therefore, visualization techniques were used to represent the data graphically as a means of gaining understanding and insight into the features within the data. This allows the researchers to more closely examine both the system and the model results, such that the data can be studied in ways that were previously difficult or impossible. The coupled arctic data have natural physical three-dimensional representations that can be usefully explored. The visualization data set includes 45 parameters, many of which are best represented spatially. These include such variables as sea-ice thickness, surface snow depth, ice concentration, flow fields, and geographic distributions of changes in velocity.

Data set size can become a computational and transfer bottleneck. For many data sets or simulations, looking at the entire data set in detail is difficult. Renderings for this project were created for 365 time-steps of 45 variables, where each variable consisted of 889,600 values resulting in ~117 GB of data to visualize.

Using an indirect geometry-based technique, structures in scalar or vector fields were visualized by converting them first into surface representations and then rendering them using conventional computer-graphics techniques. This means produces surfaces in the

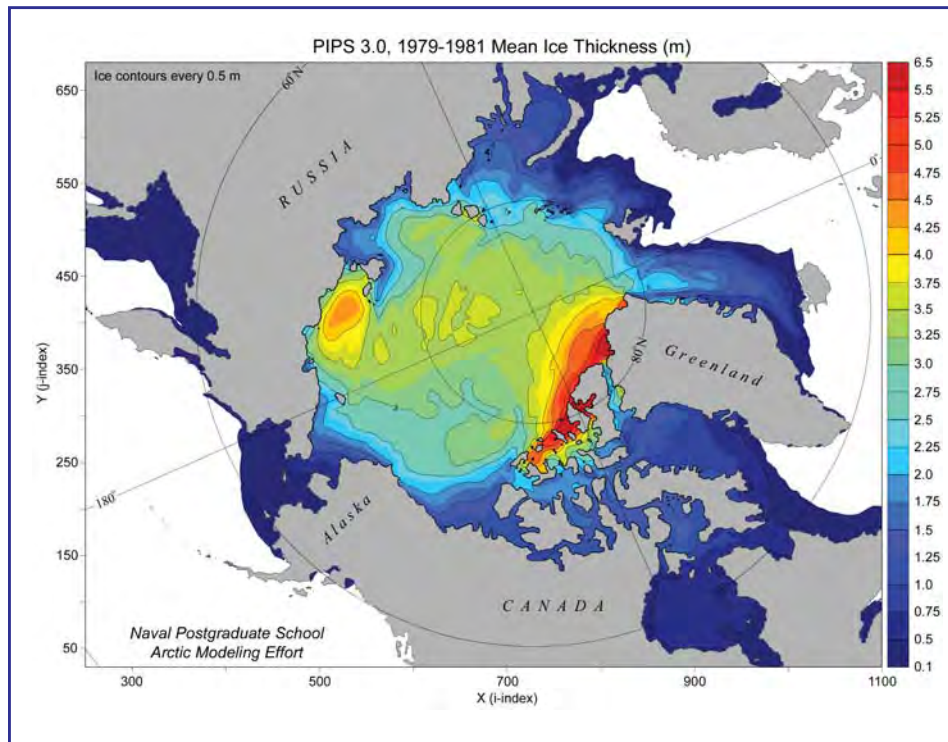


Figure 2. Three-year mean sea-ice-thickness distribution for 1979-81

domain of the scalar quantity, allowing it the same value as the surface value. Next, the surfaces can be colored according to the iso-surface value used to generate the mesh. Mapping the mesh by separate variables also gives a more unique coupled view into the data.

The method constructs a continuous surface from the discrete data set, transforming data into graphical data primitives (in this case, polygons). Graphical primitives are test rendered, and the geometrical data are converted into images. Images and extracted surfaces are then combined to produce a visualization. Textures are generated to color surfaces, e.g., those generated by the geometric-extraction techniques. A color map is used to assign the color. At the same time, reference images are created from each variable in each time-step, such that, for any specified time, a color-mapped image can be examined. Movie files were created from a sequence of rendered images of each of the variables showing the fluctuations of the values over time.

The conceptual animation team in the SVC put the scientific data into context. By modeling a SeaWolf-class submarine and rendering animations showing the vehicle emerging through a low-density section of the sea ice, the animation team enabled the researcher to view the scientific data in a useful context. An immersive interactive demonstration, which shows

annual variability in sea-ice thickness and localized fluctuations over the Arctic Region, was created for the Immersadesk for displaying the coupled ocean-climate general circulation model. The user interactively explores areas of interest in real time.

Also, a version of the Parallel Ocean Program (POP), version 2.0, written at Los Alamos National Laboratory, has been enabled to run on the Cray X1 for this specific application. Drs. John Levesque and Alan Minga of Cray, Inc., recently provided a tuned version of POP 2.0 for the ERDC Cray X1. POP 2.0 does high-resolution global and regional modeling.

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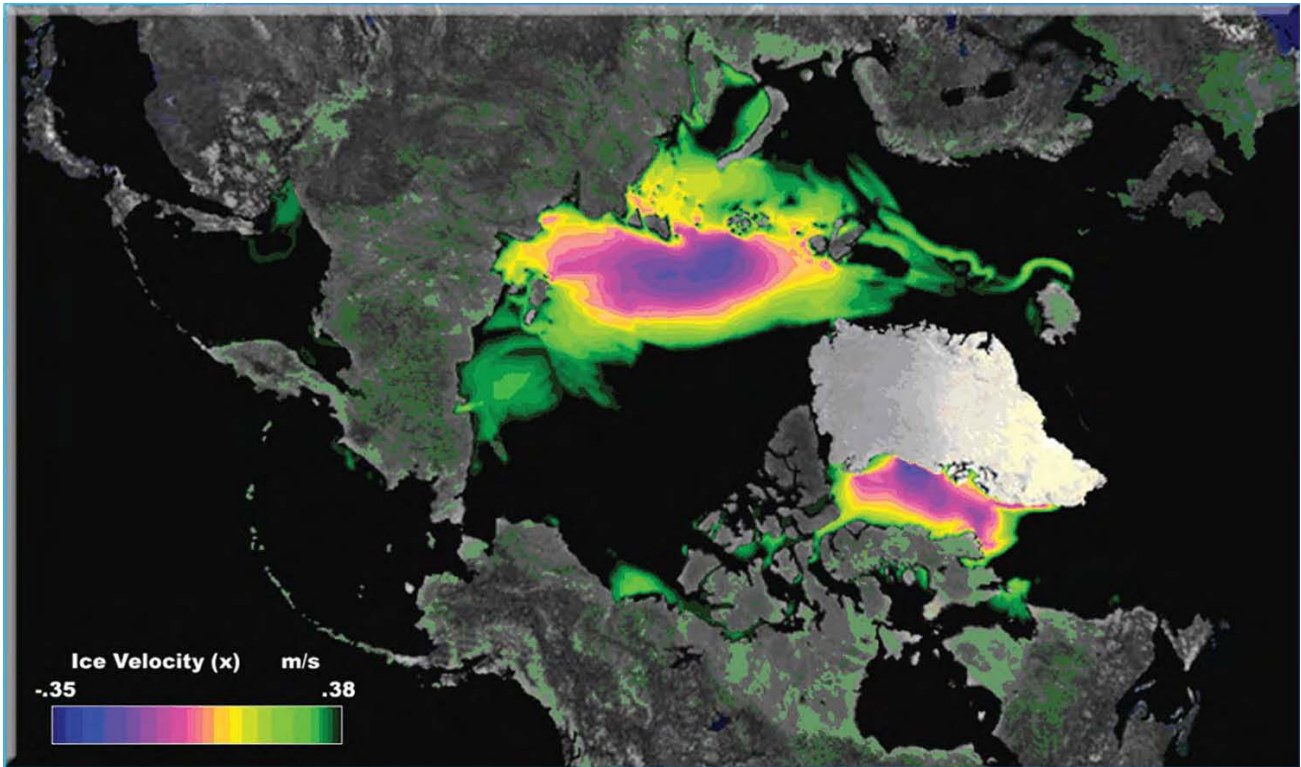


Figure 3. Ice velocity

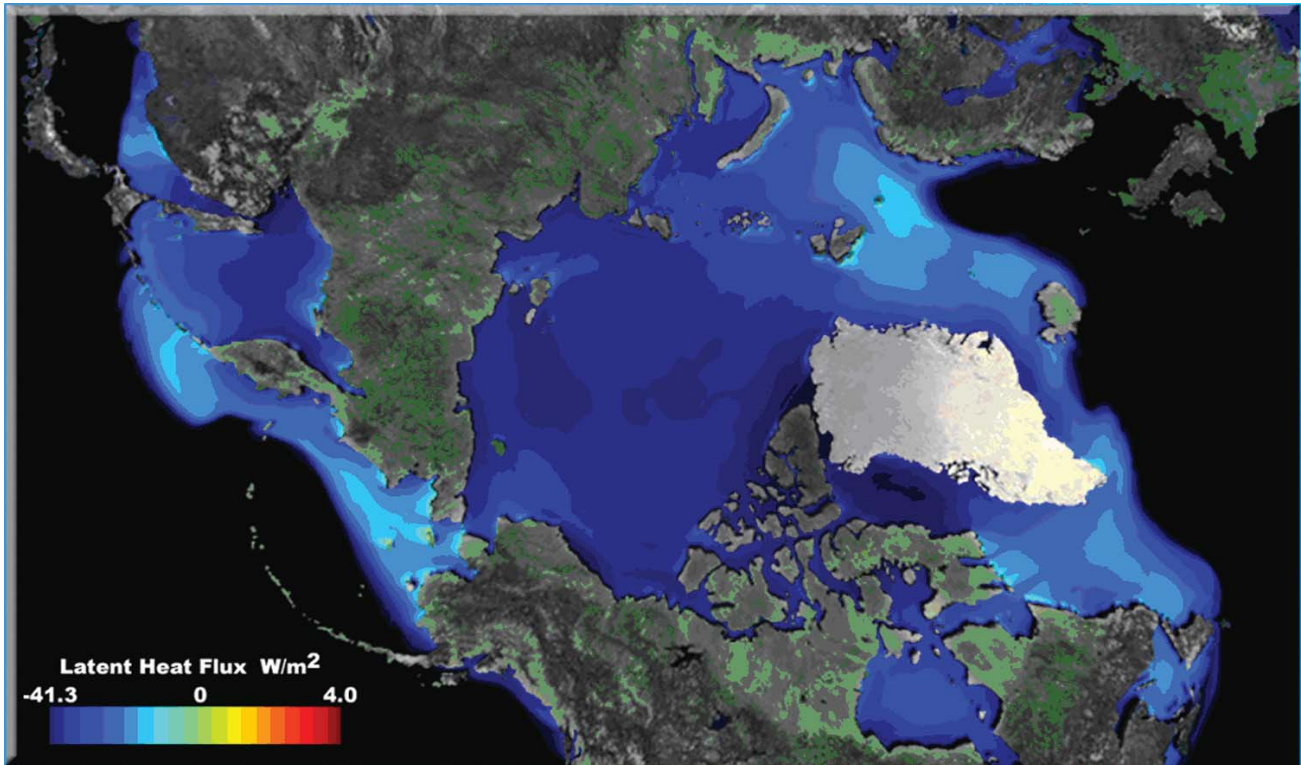


Figure 4. Latent heat flux



## **ERDC MSRC Computational Science and Engineering (CS&E) Group Creates a New Tool for Users**

By Robert M. Hunter and Dr. Ruth Cheng

A majority of scientific applications require a computational mesh, which is a discretized form of the physical domain. The mesh is represented by sets of vertices and edges, which form elements or volumes. A variety of data can be associated with the mesh, and these data can sit on vertices or elements of the mesh. When parallelism is employed, it is important to partition the mesh evenly among processors, while maintaining data coherence and low communication overhead. This can be hard. DBuilder has been developed by the CS&E staff of the MSRC to provide a simple Application Programming Interface (API) for users to sidestep the learning curve of message passing, graph theorem, and parallel algorithms. DBuilder implements these facets of parallel programming by utilizing tools and libraries such as ParMETIS (Karypis et al.) and the Message Passing Interface (MPI).

DBuilder provides support of domain partitioning, parallel data management, coupling coordination, and parallel solver interface. A mesh can be viewed as a graph  $G=(V,E)$ , which is a set of vertices ( $V$ ) and edges ( $E$ ). When a subgraph on each processor is given to DBuilder, DBuilder partitions the domain ( $G$ ) to processors. This partition may be manipulated to provide a distribution that is low in communication or a computationally balanced workload. DBuilder can build a vertex domain with a distributed number of vertices, an element domain with a distributed number of elements, or a boundary element domain comprised of boundary elements in the element domain. A vertex domain is favored when the application is to solve vertex-based values such as the finite difference method, while an element domain (or the vertex domain of the dual graph of  $G$ ) is for solving cell-centered values such as the finite volume method. As a finite element application, coordination between elements and vertices is required because the assembly procedure assembles each elemental matrix to a linear system, and the linear system is then solved for vertex-based values. DBuilder also provides a default rule for such coordination between vertices and elements. A callback approach is supported for users to specify their own rules.

Data migration among processors is encapsulated in DBuilder using MPI data types. DBuilder has the information for local and ghost vertices/elements alive throughout the entire application. This piece of information is mandatory for gather/scatter operation in the parallel paradigm. Two API functions are facilitated for the user to maintain coherent data structures among processors. MPI nonblocking functions are called in DBuilder for data synchronization.

Figure 1 shows a section of code implemented in WASH123D (Cheng et al.) to illustrate the use of the DBuilder API. In this case, both vertex and element domains are built for the finite element method to maintain a balanced number of vertices among processors. The first two function calls pass geometric information to `DBuild_Init` for building vertex and element domains, respectively. DBuilder registers their memory addresses only and does not keep a copy of the geometric information. Then, the function `DBuild_Get_file_part` can be called to retrieve the local count of data to be read on the processor. Two instances of `DBuild_Domains` are called to build the vertex domain followed by the element domain. The element domain's partition rule is based on the constructed vertex domain. These two domains have their own local entities and ghost entities, where the ghost entities are owned by other processors. Two steps are required to update data in the element array (i.e., element indices) that is not owned. These are as follows: (1) `DBuild_Set_type` is called to set the data type for the element array, and (2) `DBuild_Global_update` brings in the ghost values to the element array. Based on the DBuilder constructed element domain, some vertices may need to be available as ghosts on a given processor, because more than one ghost layer may be necessary in the algorithm. `DBuild_Add_ghosts` is available to achieve this purpose. `DBuild_Set_type` and `DBuild_Global_update` are then called to bring in the vertex coordinates for the vertex domain. At the bottom, `DBuild_Set_type` is called to set up the data type for updating the data on ghost vertices. Obviously, the data are associated with vertices because the data type is set on the vertex domain. After the domains are built, the rest of parallelization is basically to place `DBuild_Global_update` routines at appropriate locations in the code.

```
/** Initialization for vtxDomain and elementDomain */
ierr = DBuild_Init(num_global_vertices, num_ghost_layer, 0,
                  point2neighbor_list, proc_set, &vtx_neighbor_list,
                  &vtx_neighbor_list, &vtx_coord, total_bytes_of_each_vtx,
                  vtxDomain);
ierr = DBuild_Init(num_global_elements, num_ghost_layer,
                  num_neighbors_per_elm,
                  &num_entries_per_elm, proc_set, &element_array,
                  &elm_neighbor_list, NULL, 0, elementDomain);

/** Read mesh from a file --- partial file is read on each processor */
ierr = WashRead_geom3(fd, mesh); /** fill in coord and element arrays
                                  in mesh and then create neighbor list */

/** Build domains */
ierr = DBuild_Domains(1, NULL, vtxDomain);
ierr = DBuild_Domains(3, vtxDomain, elementDomain);

/** update element_array for ghost elements */
ierr = DBuild_Set_type(num_entries_per_elm*sizeof(int), &dType,
                      elementDomain);
ierr = DBuild_Global_update(element_array, dType, elementDomain);

/** add ghost vertices based on elementDomain */
ierr = DBuild_Add_ghosts(element_array, num_local_vertices,
                          num_neighbors_per_elm, num_entries_per_elm, vtxDomain);

/** bring in the coordinates for ghost vertices */
ierr = DBuild_Set_type(num_dir*sizeof(double), &dType, vtxDomain);
ierr = DBuild_Global_update(coord, dType, vtxDomain);

/** build data types for data gathering or scattering */
ierr = DBuild_Set_type(sizeof(double), &mesh->doubleType, vtxDomain);
```

Figure 1. Code containing DBuilder APIs

Multiphysics applications on multidomains have become a large focus. These applications require that multidomain integration be executed to integrate two or more applications. The spatial relationship between computational domains can be adjacent, partially/fully overlapped, or distinct. DBuilder allows for the building of a coupler object to avoid the dependency between meshes when partitioning. Figure 2 depicts the concept of this coupler implementation. In the figure, all four processors participate in two-dimensional (2-D) and 3-D simulations. Because dependency is not specified between domains when partitioning, a given processor in the 3-D domain exclusively owning a 2-D slice of the domain is not guaranteed. As shown in the figure, processor P3 owns a partition of the 2-D subdomain, which is a partition of the 3-D subdomain owned by processor P2 and P3. Likewise, the top of the 3-D subdomain that processor P1 owns is a partial subdomain partitioned to P0 and P1 in 2-D. A coupler formed with DBuilder will provide the message passing from 2- to 3-D and from 3- to 2-D as shown in the red and blue dashed arrow lines, respectively.

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Figure 3 shows a section of code used to build a vertex coupler associated with the vertex domain and an element coupler associated with the element domain. The API function `DBuild_Coupler_init` is called twice to create these two couplers. The function `DBuild_Get_coupler_size` is called for a request of the size of a coupler. The argument `DB_D2TOD1` accounts for the size of the coupler in Domain 2 (D2) when updating Domain 1(D1). From the code in Figure 3, `DBuilder` internally represents the 2-D domain as D1 and the 3-D domain as D2. This is determined by the ordering of the domains in the call to `DBuild_Coupler_init`. The function `DBuild_Coupler_update` is called to maintain consistent data on two different domains (e.g., D2 and D1) among processors. In this example, the data on D1 named `mtyp_temp`, which is a source, update the destination on D2 shown in the first argument based on the coupler's element domain mentioned at the last argument. According to the third argument, each entry being composed of two integers is known.

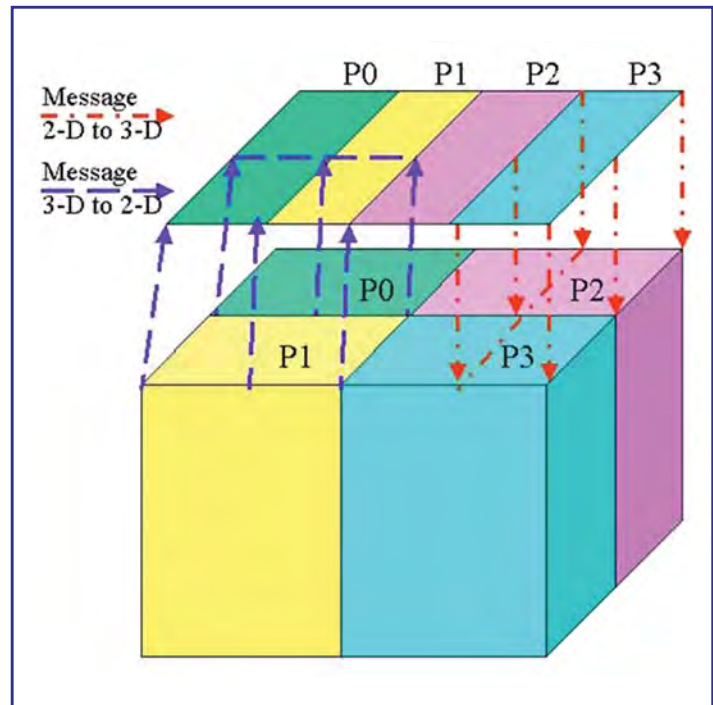


Figure 2. Concept of the coupler implementation

```
/** initialization and creation of coupler's vtx domain and element
    domain */
ierr = DBuild_Coupler_init(&mesh2->vtxDomain, &mesh3->vtxDomain,
    coupler->npxz, mesh2->vtxDomain.numberLocalElements,
    &coupler->vtx_coupler);
ierr = DBuild_Coupler_init(&mesh2->elementDomain, &mesh3->elementDomain,
    coupler->mtopxz, mesh2->elementDomain.numberLocalElements,
    &coupler->elm_coupler);

/** get the size of coupler's element domain */
ierr = DBuild_Get_coupler_size(&couplerSize, &coupler->elm_coupler,
    DB_D2TOD1);

/** update D1's vector to D2's vector on the element domain */
ierr = DBuild_Coupler_update(coupler->mtypxz, mtyp_temp, 2*sizeof(int),
    DB_D1TOD2, &coupler->elm_coupler);
```

Figure 3. Code building coupler using `DBuilder`

`DBuilder` has an interface to linear solvers such as `BlockSolve95` (Jones and Plasserman) and `pARMS` (Yousef et al.). As shown in Figure 4, only two functions are required to use the parallel linear solver `BlockSolve95`. First, `DBuild_Solver_reset_co` passes the matrix and associated geometric domain to `DBuilder`. Second, `DBuild_Solver_solve` along with the right-hand side vector, initial guess, and the associated mesh domain is passed to `DBuilder` to solve the linear system with the result stored in the second argument and the residual information at the third argument.

```
ierr = DBuild_Solver_reset_co(matrix, &mesh3->vtxDomain);
iter = DBuild_Solver_solve(rhs, x, &residual, &mesh3->vtxDomain);
```

Figure 4. Code calling `DBuilder`'s API to interface `BlockSolve95`

In summary, the full functionality of a parallel software toolkit is implemented in DBuilder. Experimental results (Figure 5) show that the overhead for building domains can be considered insignificant. However, the time spent in communication to maintain the data coherence becomes dominant as the number of processors increases. Reasons for a communication-bound application can be that the problem size is too small for a large number of processors and the parallel solver is not efficient, i.e., too much communication time spent in the solver. Thus, more sophisticated parallel solvers, such as BlockSolve95 and pARMS, are integrated into DBuilder. Figure 6 shows the performance improvement using BlockSolve95. Currently, DBuilder is installed in the `/usr/local/usp` directories on the HPC machines, and a users manual will be available shortly.

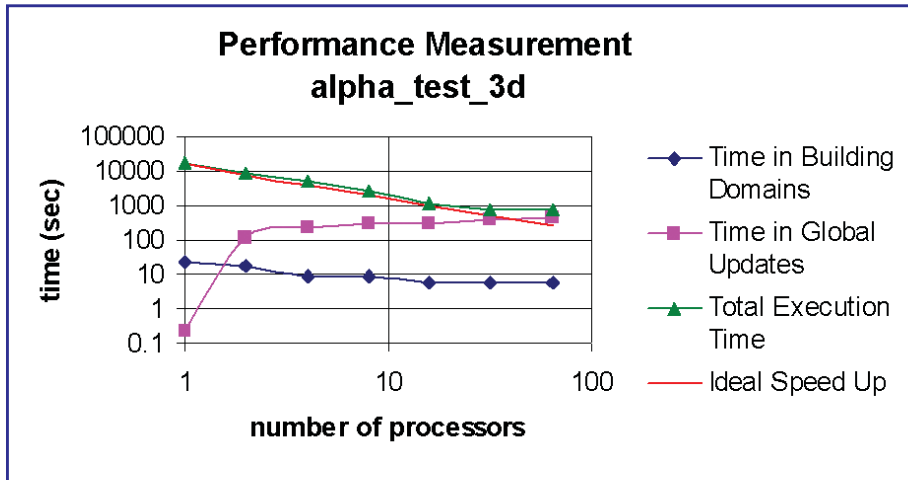
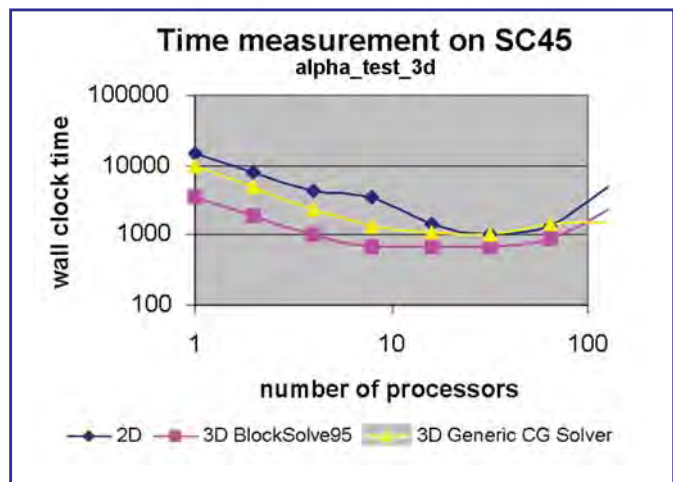


Figure 5. Performance measurement on Compaq SC45

Figure 6. Performance comparison between two linear solvers on Compaq SC45



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## ***Development of a Comprehensive Groundwater Model of the Defense Distribution Depot San Joaquin (DDJC), Sharpe Site, Lathrop, California***

*By Barbara P. Donnell, ERDC CHL, David R. Richards, ERDC ITL, Earl V. Edris, ERDC CHL, Dr. Thomas L. McGehee, ERDC CHL, and Dr. Fred T. Tracy, ERDC MSRC, ITL*

The Defense Distribution Depot San Joaquin-Sharpe, in Lathrop, California (DDJC-Sharpe), is an active military installation acting as a supply depot for the Defense Logistics Agency (see Figure 1 for a site map). It has been active for many years, and in the course of its activities, solvents used in degreasing operations have contaminated the groundwater. The primary contaminant of concern is trichloroethylene (TCE), which presents itself in three distinct plumes at DDJC-Sharpe (Figure 2). To address the contamination problem, the installation operates three pump-and-treat remediation systems to contain the three plumes and to treat the contaminated groundwater.

Until the initiation of this effort, a comprehensive groundwater model had not been developed at DDJC-Sharpe that was designed specifically to provide accurate predictions of flow and transport over a wide range of hydrologic conditions. These include such varied conditions as the siting of new municipal water wells nearby, variations in the surface-water drainage and stormwater retention ponds, and optimization of the pump-and-treat systems to get better contaminant capture for less cost.

ERDC was asked by the Huntsville Engineering and Support Center to collaborate in the development of such a groundwater model for DDJC-Sharpe (Donnell et al. 2003). The purpose of the modeling was to manage the remediation activities at DDJC-Sharpe and to determine the ultimate fate of contaminants given a variety of proposed hydrologic conditions.

Using numerical models in planning and conducting remediation operations at Department of Defense (DoD) installations has become commonplace. Indeed, a substantial investment has been made by DoD in the development of a state-of-the-art modeling system to assist in these cleanup efforts. The reasons are clear since contamination at DoD installations is significant, cleanup costs are great, and the overall DoD budget is decreasing. Modeling systems are essential for the DoD to optimize remediation and provide cost-efficient cleanup.

While numerical models have a broad range of uses, narrowly focusing the purpose of the modeling exercise is important. One modeling approach is not appropriate for all sites, just as treatment technologies



**Regional Map for DDJC-Sharpe and DDJC-Tracy Installation Locations**

*Figure 1. Site map of the region of interest*

for contamination are site specific. Modeling does not solve all problems at a cleanup site but does indeed improve the chance for remediation success.

The specific purpose of this modeling exercise is to develop a regional scale model that can address a wide range of groundwater management questions. The developed model will be housed within a graphically driven user environment that will allow the installation to add data as they are collected and to build a “living” groundwater model of the installation. The system will be “living” in that it will exist as an integral part of the remediation management plan throughout its life.

The model will continue to improve through time as additional data or model improvements are added. With these additions, the model accuracy will improve as will its adaptability; and, therefore, remediation effectiveness will be easier to demonstrate. Ultimately, the performance of the remediation action and the model’s ability to forecast this behavior will be crucial in managing the treatment practices over the remaining

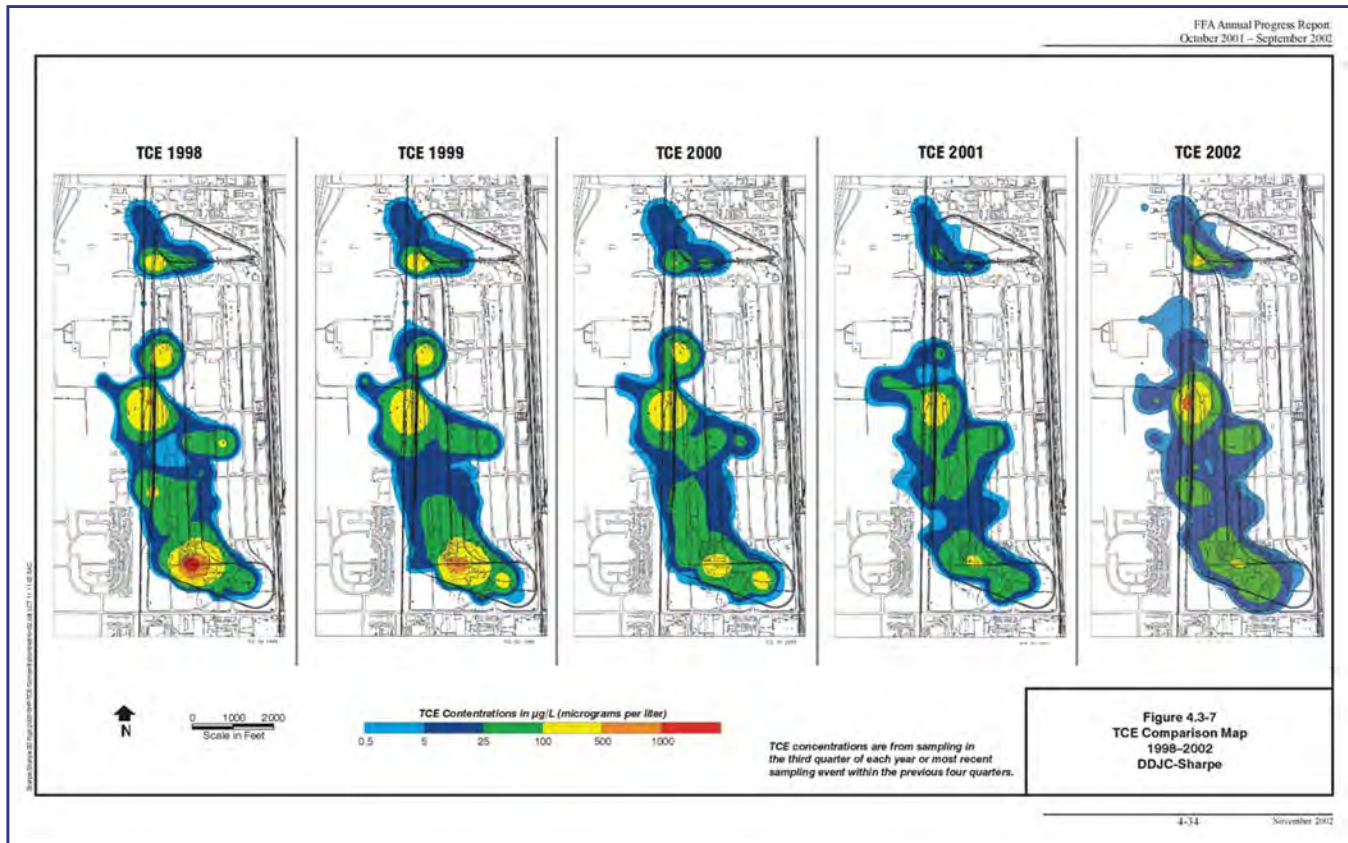


Figure 2. North Balloon, Central area, and South Balloon historical TCE concentration contours at the DDJC-Sharpe site. Concentration data and figure provided by URS Corporation, the onsite contractor

life of the remediation project. This includes the predictions to questions of when to end pumping and what potential benefits will be realized from natural attenuation of the contaminants.

The modeling system chosen for the DDJC-Sharpe application is the DoD Groundwater Modeling System (GMS) (Groundwater Modeling Team 2004). GMS was designed and constructed precisely for the type of application presented at DDJC-Sharpe. GMS contains a wide variety of database, conceptualization, visualization, simulation, and optimization tools to develop remediation designs and manage remediation efforts.

Unstructured finite element models such as FEMWATER (Lin et al. 1997) are more useful in complicated geometric settings. Numerically, a need for mesh resolution flexibility exists at DDJC-Sharpe since the location and number of wells or surface-drainage features could be changed dramatically from one simulation to the next. Since many wells can be simulated, with each well providing a potentially steep cone of depression, a need to apply higher grid resolution only where the gradients occur exists. FEMWATER also has the advantage of variably saturated, coupled flow and transport.

For these reasons, the numerical model selected for application at DDJC-Sharpe was FEMWATER. FEMWATER was originally put into the GMS with support provided by the U.S. Environmental Protection Agency (USEPA), Region IV. The reason for its inclusion was to address complexities in groundwater flow problems not suitably addressed in other models.

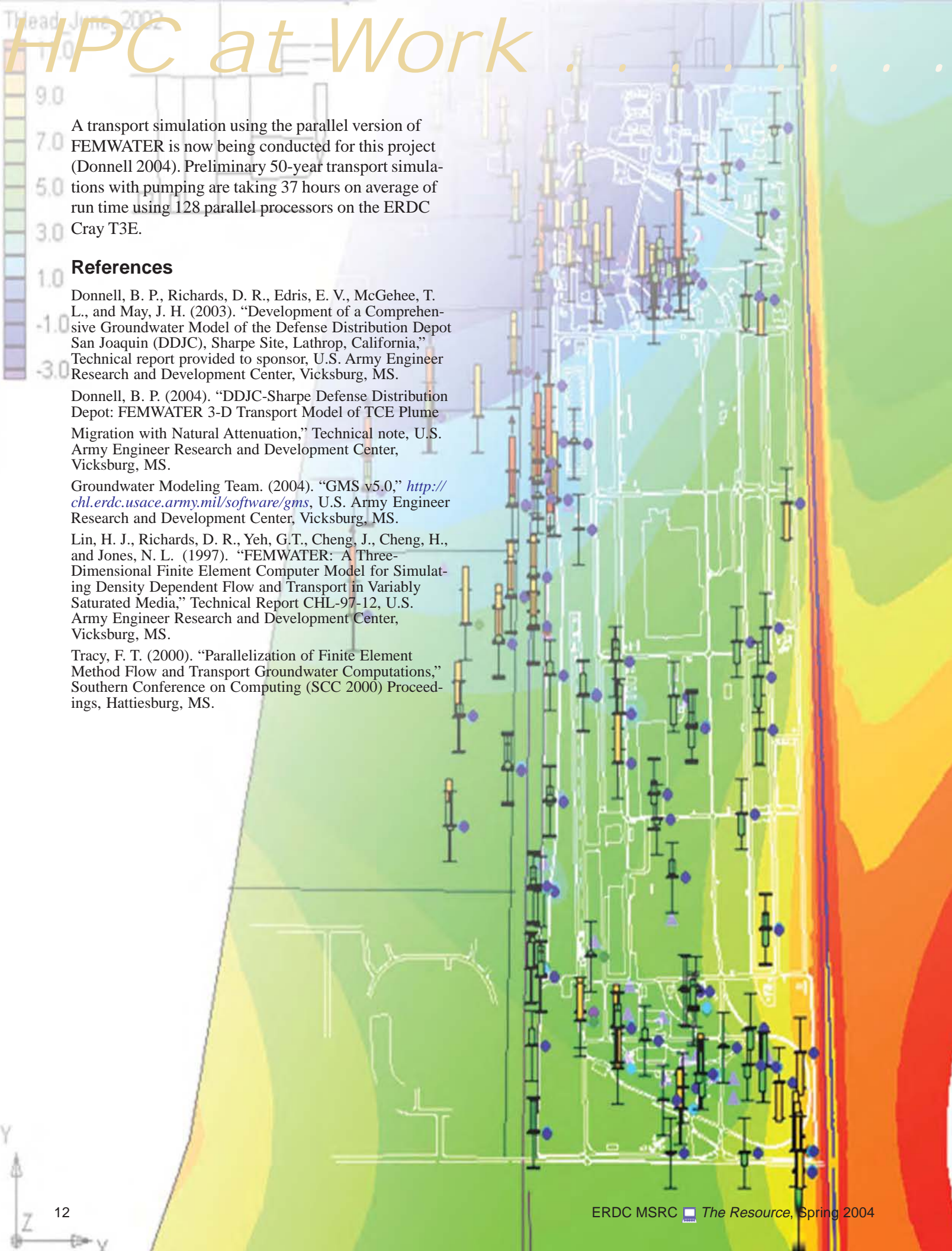
FEMWATER has been converted to the parallel computational environment (Tracy 2000). This provided the production tool to accurately model complex unsaturated groundwater problems such as the percolation pond scenarios. In order to conduct large-resolution simulations, a parallel computational environment, such as the ERDC Cray T3E, was required. This technology provides the capability to divide a large problem into a discrete number of smaller problems that can be simultaneously solved on a set of processors. Quality control measures were conducted to ensure comparability between the serial and the parallel versions of FEMWATER. On average, approximately 22 minutes was the run time for 64 parallel processors to solve the steady-state flow simulations needed as compared with 13 hours on an available serial workstation.

# HPC at Work

A transport simulation using the parallel version of FEMWATER is now being conducted for this project (Donnell 2004). Preliminary 50-year transport simulations with pumping are taking 37 hours on average of run time using 128 parallel processors on the ERDC Cray T3E.

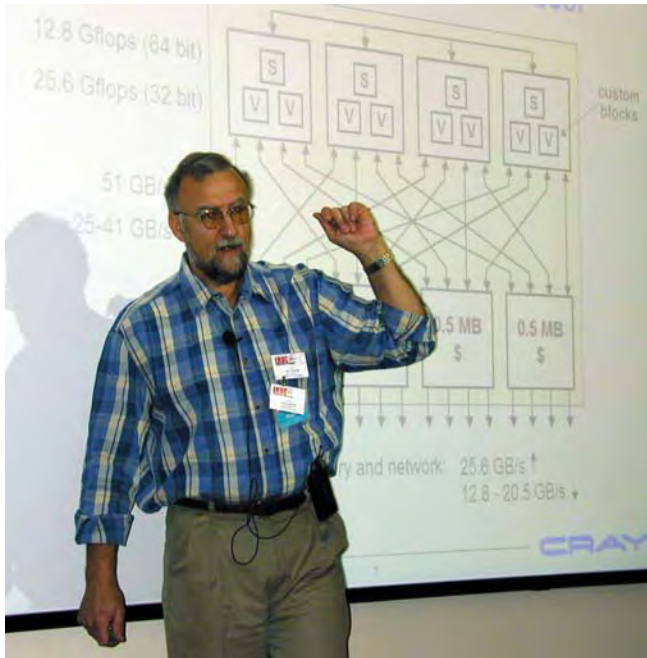
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## Cray X1 Impact

By Dr. Paul M. Bennett, Robert Alter, and Dr. Fred Tracy



*Dr. John Levesque, a Cray Applications Specialist, served as an instructor at the ERDC MSRC's Cray X1 "Bring-Your-Own-Code" workshop*

## Cray X1 "Bring-Your-Own-Code" Workshop

The ERDC MSRC hosted a "Bring-Your-Own-Code" workshop for users new to the Cray X1 architecture on March 2-4, 2004. The Cray X1, a liquid-cooled, multi-streaming vector supercomputer, was delivered to the ERDC MSRC in June 2003 and became fully available to users on January 1, 2004. Its peak computational performance of 800 billion floating-point operations per second (Gflop/s) is provided by 64 multistreaming processors, each containing four single-streaming processors and 4 GB of RAM, for a total of 256 GB of memory. Topics discussed at the Cray X1 workshop, held in the ERDC Information Technology Laboratory Collaboratorium, included hardware design, techniques for porting and optimizing codes, parallel-ization techniques, compiler features, tools for debugging and performance analysis of codes, and a Portable Batch System (PBS) for submitting jobs and determining job status. The workshop was organized and led by Dr. Paul Bennet of the ERDC MSRC. Dr. John Levesque of Cray described X1 architecture and programming

techniques. Dr. Fred Tracy of the ERDC MSRC gave a presentation on graph coloring strategies that allow multistreaming, and Dr. Andrew Johnson of the Army High Performance Computing Research Center (AHPCRC) gave a presentation on his CFD code. Participants included representatives from the major services and agencies that compute in the High Performance Computing Modernization Program (HPCMP) from sites across the country. The primary focus of the workshop was to assist users in immediately migrating their codes to the X1 and then tuning them for better performance. Members of the ERDC MSRC's Computational Science and Engineering (CS&E) group were paired with user attendees to accomplish this, and significant progress was made on most of the codes. The workshop was so well received that the ERDC MSRC is planning future workshops to further facilitate the X1 code migration process.



*Dr. Steve Ketcham, far right, of the ERDC CRREL, received excellent results with PTOP3D at the ERDC MSRC's Cray X1 "Bring-Your-Own-Code" workshop*



# HPC at Work . . . . .

## More Cray X1 Impact

Dieter Postl, a doctoral candidate working with Dr. Herman Fasel of the Department of Aerospace and Mechanical Engineering at the University of Arizona, is using NST3DD to perform computational fluid dynamics (CFD) simulations of low-pressure turbulent flows for various generic geometries. NST3DD solves the time-dependent incompressible Navier-Stokes equations using a pseudo-spectral method with Fourier components in the z-direction and compact 4th-order finite differences in the x- and y-directions. The code was originally parallelized across the Fourier modes using OpenMP. However, the high-memory bandwidth causes scaling to rapidly deteriorate for more than four CPUs. The code was migrated to a vectorized multi-streamed MPI code on the Cray X1, whose large internode and intranode memory bandwidth allows much more rapid processing. Recent computations requiring roughly 82 million grid points on 10 nodes of the Cray X1 have had turnaround time less than 24 hours, compared with longer than 3 months on an SGI Origin 3400.

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**Recent computations requiring roughly 82 million grid points on 10 nodes of the Cray X1 have had turnaround time less than 24 hours, compared with longer than 3 months on an SGI Origin 3400.**

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## *New Data Translator Enables Visualization of CTH Results with the General Mesh Viewer*

By Dr. Richard A. Weed

The CTH hydrocode developed at Sandia National Laboratory is one of the standard tools used by Department of Defense (DoD) researchers for explosive effects analysis and force protection design. An essential part of any CTH analysis is the visualization of results at various times in the simulation cycle to determine the current status of simulation. In addition, visualization tools that can display all or part of a simulation interactively in three dimensions are required for determining where problems might be occurring in the simulation. However, the visualization tools supplied with CTH are based on two-dimensional graphics packages that do not allow users to interact with the data in three dimensions. CTH users at several DoD sites in discussions with members of the HPCMP Programming Environment and Training (PET) program Computational Structural Mechanics (CSM) team identified enabling visualization of CTH data with widely available three-dimensional (3-D) visualization tools. Two of these tools are TECPLOT and the General Mesh Viewer (GMV) program from Los Alamos Laboratories as a potential PET core support activity. Based on these requests by DoD users, the development of a series of data translators that can convert CTH data into formats readable by several different visualization tools was undertaken by PET.

The decision was made that the first of these translators would be targeted at generating data that could be viewed with the GMV program since GMV is freely available, noncommercial software that runs on a wide variety of UNIX workstations and HPC systems. Therefore, it can be installed on individual user workstations without the expense of a software license. In addition, GMV is currently used by researchers at ERDC to visualize results from another hydrocode (SHAMRC). GMV is an OpenGL application with a wide variety of features for viewing data generated by Finite Element and Finite Volume codes interactively in three dimensions. These features include support for most of the commonly used finite element shapes, cut planes, rendering of iso-surfaces and iso-volumes, and viewing multiple material data. In addition, a parallel version of GMV exists for batch rendering of large data sets. Since the GMV viewer can distinguish between the internal binary data formats of different systems, GMV data files can be created on any HPC system and viewed on user local workstations without external translation of the data file into the

internal binary format of the workstation.

Development of a CTH to GMV translator was begun in 2003. After reviewing the FORTRAN 77 code used by CTH to create restart and plot data files, the decision was made that the basic routines required to read CTH data files would be rewritten in FORTRAN 95 to enhance code portability and long-term maintainability. This approach also eliminates the need to have access to the CTH code base and libraries for users who would like to build their own versions of the data translators. In addition, a library of C utilities provided by Los Alamos for creating GMV files was also implemented in FORTRAN 95 along with a small library of C utilities of FORTRAN-compatible wrappers around C intrinsic functions required to create C stream data format files used by GMV. The resulting code base for the translator is predominately FORTRAN 95 code with only a small percentage of the required code written in C. This eliminates many of the problems associated with migrating mixed FORTRAN and C applications across different hardware platforms. In addition, most, if not all, of the nonstandard conforming code used in the CTH FORTRAN 77 routines such as dynamic memory allocation using CRAY pointers can be replaced by FORTRAN 95 code that rigidly adheres to the FORTRAN 95 standard. The plan is that all of the C code currently used to access the underlying C I/O utilities will be replaced with logic that conforms to the C interoperability features proposed for the forthcoming FORTRAN 2003 standard that is scheduled for final approval in 2004.

A beta version of the CTH to GMV data translator named CTH2GMV was released for public review in January of 2004. The beta version is a scalar application that supports reading of both single-processor and parallel CTH data files. Users can select specific CTH variables to dump at user-specified time-steps. Most of the variables that can be plotted with the existing CTH visualization programs can be extracted by CTH2GMV. User input for CTH2GMV is based on a simple keyword-oriented format that duplicates many of the keywords used for existing CTH inputs. Much effort was devoted to keeping the required input to a minimum. The following example illustrates all of the data required to extract cell pressure for all of the CTH time-steps stored in multiple CTH plot files (plcth) generated by a parallel run and create a GMV file with

# HPC at Work . . . . .

a root file name of run1\_p for each time-step that contains the requested data.

CTH2GMV input example:

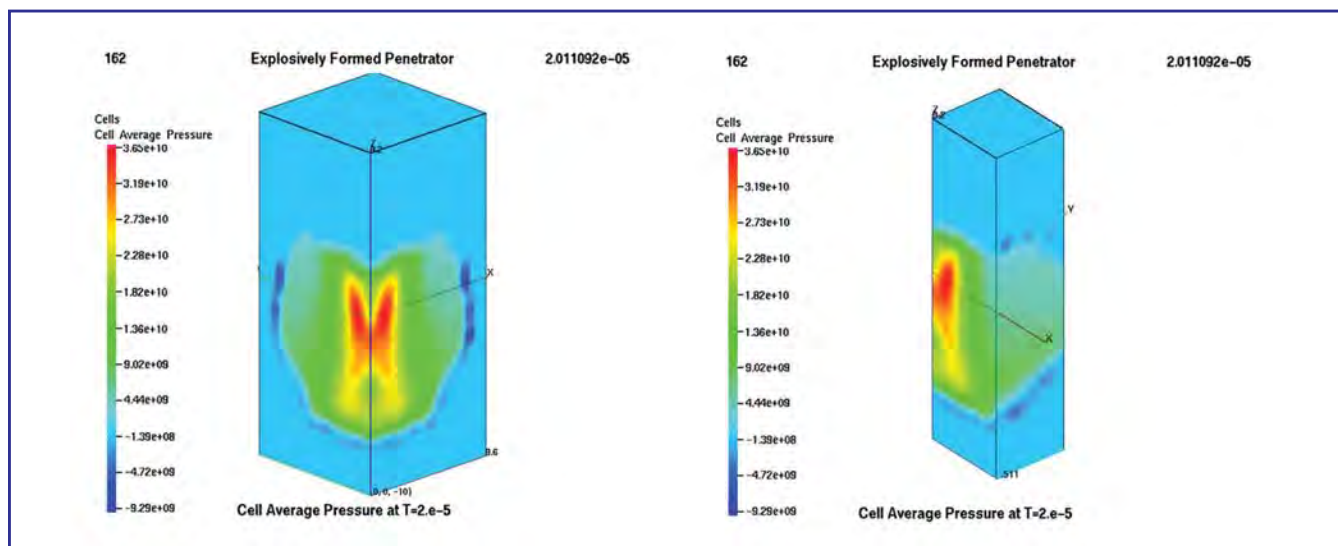
```
$ /usr/local/usp/CTH02/CTH2GMV/bin/cth2gmv  
CTH2GMV > mf=plcth gf=run1  
CTH2GMV > get all var=p  
CTH2GMV > quit
```

CTH2GMV also supports writing multiple variables to each GMV input file. In addition, three data decimation procedures can be selected to reduce the size of the output data and restrict the region of the CTH grid from which data are extracted. CTH2GMV can read both CTH restart and plot (plcth) files.

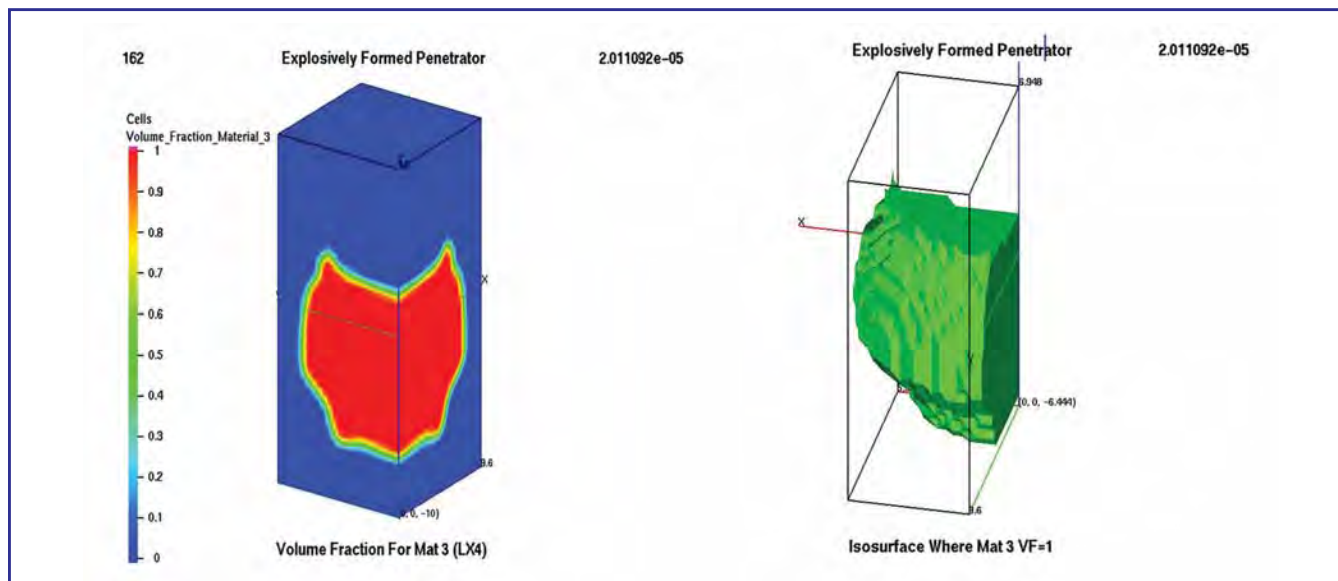
Development of CTH2GMV is still ongoing with final release planned later in 2004. A parallel MPI-based version of the code is planned for the final release along with support for simulations that used Adaptive Mesh Refinement. In addition, future translators are planned to support TECPLOT and the SANDIA EXODUS database format.

The beta-release version can be accessed by members of the CTH group on the ERDC COMPAQ SC40/45 and SGI ORIGIN systems. ERDC MSRC CTH users interested in trying out CTH2GMV should contact Dr. Richard Weed ([Richard.A.Weed@erdc.usace.army.mil](mailto:Richard.A.Weed@erdc.usace.army.mil)), ERDC PET Onsite Lead for CSM, for more details on accessing and running the code.

*The following figures illustrate CTH pressures on the symmetry planes and interior cut planes generated by the detonation of an explosively formed projectile*



*The next figure illustrates volume fraction contours for the explosively formed projectile simulation*



## EasyHPC Debuts in Beta Test

High performance computing is on its way to becoming easier, thanks to a new Web-based utility developed by the Software Engineering and Evaluation Branch of the Engineering and Informatics Systems Division in ITL in partnership with the ERDC MSRC. EasyHPC allows users to upload/download files, manage and submit batch jobs, cancel jobs, display job statistics and CPU usage, and provide command line execution

to the ERDC MSRC parallel computers from the comfort and familiarity of their normal desktop environment. The EasyHPC Beta, targeted initially at Windows users, entered beta evaluation with a small group of HPC users on April 13, 2004. The Beta Review Team is advising the development group on final tweaks to the software before general distribution, expected later this fiscal year.

## tips and techniques

### Simple Techniques for Improving Performance - Case Study

By Bobby Hunter

The Deformation Mapping Technique (DMT), a serial code that identifies deformations induced from stresses applied to a specimen, has been recently improved. The technique compares pixels in a digital image taken before the straining event with a digital image taken afterwards. The technique knows no scale boundaries and can be applied to deformation at the microscopic level as well as at the macroscopic level. This enables deformation imaging of a range of scales, from large structures such as buildings and bridges to micrometer-sized points in an experimental specimen. Total runtime on example executions on the ERDC MSRC's Origin 3900 was reduced from 37,000 to 51 seconds, an improvement of 725-fold. This parallelization and optimization process permits more images to be analyzed in a given time frame at a reduced cost to process the data and enables researchers to analyze material deformation to a greater depth. As a result, 10 image pairs can now be analyzed in 1 day compared with the previous metric of one pair in 2 days.

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**As a result, 10 image pairs can now be analyzed in 1 day compared with the previous metric of one pair in 2 days**

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Reducing wall clock time from 37,000 to ~7,000 seconds, without code modifications, was done by using compiler optimizations. The code was compiled with -O3 flag passed to the compiler, which turns on aggressive optimization. Floating point accuracy may be affected as the compiler rearranges floating-point instructions, resulting in rounding variances from the nonoptimized code. Also, the compile time will increase as the compiler generates high-quality code. To ensure that the -O3 code generated acceptable results, the output from the code built with optimiza-

tions was validated against output results from nonoptimized code. For this particular case, the O3 results were deemed acceptable as long as the maximum difference between the O3 results and O0 results was no greater than 10e-6.

DMT was an exceptional candidate for parallelization, as it was embarrassingly parallel. By this, it means that the data could be divided into independent "subdata" blocks and the same computation performed for each subdata block on an independent processor. Therefore, a processor could work on a given portion of the grid without a need for interaction with other processors. The only parallel logic needed was to determine on which points of the grid each processor would work. For this particular problem, the grid was divided into column strips for distribution across processors. The following code snippet demonstrates the algorithm executed by each processor for determining the strips that it would compute.

```
MPI_Init(&argc, &argv);
MPI_Comm_size(MPI_COMM_WORLD, number_processors);
MPI_Comm_rank(MPI_COMM_WORLD, my_process_id);
remainder = total_points_x % number_processors;
my_number_points_x = total_points_x / number_processors;
if (my_process_id < remainder)
    my_number_points++;
my_start_point_x = my_number_points_x * my_process_id;
if (my_process_id >= remainder)
    my_start_point_x += remainder;
```

Only four calls to the Message Passing Interface (MPI) were essential in parallelizing the code; three of these are included in the above code:

```
MPI_Init()
MPI_Comm_size();
MPI_Comm_rank();
MPI_Finalize();
```

MPI-IO routines were used for parallel output of the solution but were not a necessity. For more information on MPI routines, visit <http://www.mpi-forum.org>.

## *The ERDC MSRC Challenge Projects Support Team*

*By Dr. Paul M. Bennett*

Each year, the Deputy Under Secretary of Defense for Science and Technology, together with the Director of the DoD High Performance Computing Modernization Program (HPCMP), selects Challenge Projects for allocations on the total HPC resources provided by the HPCMP. Each Challenge Project may run for up to 3 years, with possible extension for another 6 months.

The ERDC MSRC has been assigned 19 of these Challenge Projects for FY2004. These Challenge Projects account for roughly 10 percent of the total hours available at the ERDC MSRC. The projects are as follows:

- Directed High Power RF Energy: Foundation of Next-Generation Air Force Weapons
- High Fidelity Analysis of UAVs Using Non-Linear Fluid Structure Simulation
- High Fidelity Simulation of Littoral Environments
- Seismic Signature Simulations for Tactical Ground Sensor Systems
- Multiscale Simulations of Nanotubes and Quantum Structures
- Multiscale Simulations of High Energy Density Material
- Evaluation and Retrofit for Blast Protection in Urban Terrain
- First Principal Studies of Technologically Important Smart Materials
- Numerical Modeling of Turbulent Waves for Naval Applications
- 3-D CFD Modeling of the Chemical Oxygen-Iodine Laser II
- Simulation of Coherent Radar Backscatter from Dynamic Sea Surfaces
- 3-D Modeling and Simulation of Weapons Effects for Obstacle Clearance
- Computational Support for Chemically Reactive Flows and Non-Ideal Explosives
- Stochastic Simulations of Flow Structure Interactions
- Towards Predicting Scenarios of Environmental Arctic Change
- Scalable Simulations of Combustion Chamber Dynamics and Hypergolic Gel Propellant Chemistry for Selectable Thrust Engines in Next-Generation Guided Missiles
- Tip-to-Tail Turbulent Scramjet Flowpath Simulation with MHD Energy Bypass
- High Accuracy DNS and LES of High Reynolds Number, Supersonic Base Flows, and Passive Control of the Near Wake



*ERDC MSRC Challenge Projects POCs: (seated left to right) Dr. Paul Bennett, Chris Fuson, Bobby Hunter, Carrie Leach, Dr. Nathan Prewitt, and Bob Alter; (standing left to right) Tommy Biddlecome, Paul Adams, Mike Gough, Richard Walters, Dr. Sam Cable, and Dr. Fred Tracy. (Not pictured are Phil Bucci, Dr. Jeff Hensley, Dr. Tom Oppe, Bill Renaud, and David Sanders)*

The ERDC MSRC assists its Challenge Projects with a team of Points-of-Contact (POCs) comprised of Government and contractor employees. The Challenge Support Team includes members of the Computational Science and Engineering group, the Scientific Visualization Center, the Programming Environment and Training (PET) program team, and the Customer Assistance Center. Dr. Bennett is the ERDC MSRC Challenge Projects Coordinator. The Challenge Projects Support team monitors the progress that the Challenge Projects make against their allocations and works closely with the ERDC MSRC Customer Assistance Center to resolve any issues that may impede performance of the Challenge computational tasks. The team also assists with code migration and tuning.

Communication plays a vital role in resolving issues and monitoring the Challenge Projects. The Challenge Projects Coordinator regularly reviews system issues and the status of each Challenge Project. The POCs meet regularly to discuss the status of their respective Challenge Projects and any issues or problems that the Projects may have. Additionally, the Coordinator meets with each POC as needed to discuss and resolve issues requiring greater attention, such as software purchases, allocation reimbursements, or hardware problems. This approach allows the Challenge Projects Support Team to support the ERDC MSRC Challenge Projects with a high level of success.

For more information regarding the Challenge Projects at the ERDC MSRC, please contact Dr. Paul Bennett through the Customer Assistance Center at [msrchelp@erd.c.hpc.mil](mailto:msrchelp@erd.c.hpc.mil) or telephone 1-800-500-4722.

## *Honing the Edge*

*By Gerald R. Morris*



*Rikk Anderson discusses pipeline hazard mitigation techniques*

As part of the continuing effort to provide professional development opportunities to its staff, the ERDC MSRC is undertaking a seminar series on computer architecture. The intent is to give ERDC MSRC staff members detailed insight into the inner workings of modern digital computers. The seminars, which are being facilitated by Dr. Bill Ward, ERDC MSRC Computational Science and Engineering lead, began in January 2004 and will continue through December 2004. Each participating member is responsible for preparing and presenting a seminar on some computer architecture topic. Topics span the entire range of computer architecture, including fundamentals of computer design, instruction set architectures, pipelining, memory hierarchy, multiprocessors, storage systems, and interconnection networks. The textbook used for the seminar series is Hennessy and Patterson's classic text, *Computer Architecture: A Quantitative Approach*, 3rd Edition.

## Supercomputing 2003 “Igniting Innovations”

By Rose J. Dykes

The Phoenix Civic Plaza Convention Center, Phoenix, Arizona, was the site of the 15th supercomputing conference. Highlighting the most innovative developments in high performance computing and networking, SC2003 brought together researchers, engineers, scientists, educators, etc., presenting projects that they had in the works and computer hardware and software vendors showing off their wares.

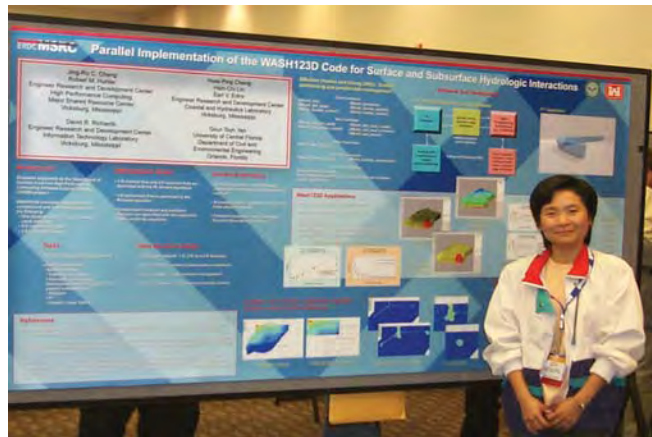
TeraFLOPS-level machines presented at this conference have come a long way from when peak performance was an “impressive” 3 gigaFLOPS at the first SC conference held in Orlando, Florida, in 1988. This conference has highlighted important innovations of the information age starting with the birth and growth of the World Wide Web.

Dr. Ruth Cheng represented the ERDC MSRC at the conference technical program with her presentation of a poster entitled “Parallel Implementation of the WASH123D Code for Surface and Subsurface Hydrologic Interactions.” Paul Adams and Richard Walters presented scientific visualization lectures as well as demonstrations. Robert Athow and Dr. Wayne Mastin explained the PET program to booth visitors.

The NAVO MSRC was tasked with the responsibility for the DoD HPCMP booth for SC2003. Work has already begun at ERDC for the SC2004 Conference to be held in Pittsburg, Pennsylvania, November 6-12, 2004. The ERDC MSRC will be heading up the DoD HPCMP booth this fall, supporting the SC2004 “Bridging Communities” theme.



Dean Hampton (center), ERDC MSRC, and Dr. George Heburn (far right), Mississippi State University, answer questions at the DoD HPCMP booth



Dr. Ruth Cheng at the Conference Poster Session



Professor Shahrouz Aliabadi (left), Clark Atlanta University, and Robert Athow, ERDC MSRC, at the HPC in Mississippi booth

## ***Department of Energy Computer Graphics Forum***

Paul Adams, ERDC MSRC Scientific Visualization Lead, made a presentation entitled “Large-Scale Visualizations of Department of Defense Challenge Projects” at the Department of Energy Computer Graphics Forum in Santa Fe, New Mexico, on April 27, 2004. He discussed the process by which visualization of these large-scale simulations is performed. Over 60 people attended the forum from various national laboratories including those from Los Alamos, Lawrence Livermore, and Sandia, and the High Performance Computing Modernization Program (HPCMP) centers. The goal of scientific visualization is enabling the DoD researchers to discover phenomena occurring in the simulation that they had previously not been able to observe. The expertise of the Scientific Visualization team is available to users of the HPCMP computing resources.

## ***ERDC MSRC Video Winning Entry at American Physical Society Meeting***

An ERDC MSRC user, Antonino Ferrante, in conjunction with Paul Adams, Miguel Valenciano, and David Longmire of the Scientific Visualization Center presented a video at the 56th American Physical Society (APS) meeting, Division of Fluid Dynamics. The video was among the four winners of the Gallery of Fluid Motion videos at the APS-DFD 2003. The video was entitled “Evolution of Quasi-Streamwise Vortex Tubes and Wall Streaks in a Bubble-Laden Turbulent Boundary Layer over a Flat Plate.” The visualization showed resulting vortex tubes from the direct numerical simulation of turbulent flow over a flat plate. The video was shown at the American Physical Society meeting in March, and a short article will appear in the *Physics of Fluids* journal in September 2004. It will then be placed on the Web site of the APS Gallery of Fluid Motion (<http://www.aps.org/units/dfd/index.html>).

## ***“Maxwell’s Equations” Paper Published in Elsevier Journal Physica D***

Dr. Paul Bennett, ERDC MSRC, and Dr. Alejandro Aceves, University of New Mexico Department of Mathematics and Statistics, published the paper “Parallel Numerical Integration of Maxwell’s Full-Vector Equations in Nonlinear Focusing Media” in *Physica D*, Vol. 184, pp 352-375, October 1, 2003. This paper presents results of parallel numerical integration of Maxwell’s equations in bulk Kerr glass. The index of refraction of Kerr materials depends upon the intensity of the coherent light. In this study, ultra-short optical pulses of light were propagated through a regular rectangular grid in order to study the distance to blowup of sufficiently intense pulses.

## ***IEEE Visualization 2003 Conference***

Paul Adams, ERDC MSRC Scientific Visualization lead, presented a paper at the IEEE Visualization 2003 Conference in Seattle, Washington, on October 23, 2003. The paper was entitled “Visualization of Steep Breaking Waves and Thin Spray Sheets Around a Ship.” The Simulation and Visualization of the Breaking of Waves, the Formation of Thin Spray Sheets, and the Entrainment of Air Around the Next Generation of Naval Surface Combatants is an ongoing 3-year DoD Challenge project. The goal of this project is to develop a validated computation capability to model the full hydrodynamics around a surface combatant, including all of the processes that affect mission and performance. The novel visualization of these large-scale simulations enabled the researchers to discover phenomena occurring in the simulation that they had previously not been able to see.

## ***SIAM Conference on Parallel Processing for Scientific Computing Participation***

Drs. William A. Ward, Jr., and Ruth Cheng, both with the ERDC MSRC, made presentations at the Society for Industrial and Applied Mathematics (SIAM) Conference on Parallel Processing for Scientific Computing. The conference was held February 25-27 in San Francisco, California. Dr. Cheng presented a paper entitled “Development of Parallel Particle Tracking Algorithms in Large-Scale Unsteady Flows.” Her presentation focused on the development of an Ordinary Differential Equation solver to solve trajectory equations in unsteady flows. The application of the overland flow problems solved by the diffusion wave model was demonstrated.

Dr. Ward’s presentation, “Experiences Profiling and Characterizing DoD High Performance Computing Applications,” defined the goals of gathering profile data for the HPCMP profiling project, identified the three levels of profiling to be used to characterize the computational behavior of DoD HPC applications, and described the benchmark application codes analyzed by the MSRC for the HPCMP office.



# Shaping the future . . .

## ***A Joint Outreach Effort of the ERDC and NAVO MSRCs Expands Awareness of High Performance Computing in the State of Mississippi***

By Rose J. Dykes

ERDC MSRC Director John E. West and NAVO MSRC Director Stephen A. Adamec spoke at the inaugural session of the 2003-04 Evening Seminar Lecture Series on High Performance Computing, one part of an ongoing effort between the Department of Defense and various universities in Mississippi. The primary goal of the lecture series was to increase awareness of HPC within the State of Mississippi, through focused efforts among DoD, academia, and private industry.

West and Adamec presented talks at the University of Southern Mississippi (USM) on October 23 that complemented one another, with Adamec presenting perspectives on present and future HPC capabilities and West focusing on HPC applications of the research challenges facing supercomputing in the future. The session, geared toward preparing the next generation of science, engineering, and HPC workers, was attended

by more than 150 students and faculty. Extensive question and answer periods were held after both talks.

On February 26, Paul Adams, ERDC MSRC Scientific Visualization Center, and Pete Gruzinskas, NAVO MSRC Scientific Visualization Center, both spoke on HPC for scientific visualization at USM and then again on the same topic at Jackson State University (JSU) on March 11.

West spoke again at JSU on March 4 about the user perspective on HPC and how to prepare for careers in HPC. On March 25, Jay Cliburn, ERDC MSRC Technical Operations Manager, ended the lecture series with a presentation entitled “High Performance Computing: An Operations Manager’s Perspective” at USM. His presentation included an overview of parallel computing and various HPC architectures.

## ***Vicksburg High School Students Shadow ERDC MSRC Team Members***

Students from Vicksburg High School, Vicksburg, Mississippi, recently visited ERDC to shadow ERDC team members that work in fields in which they are interested. Dr. Bill Ward and Paul Adams both of the MSRC participated in this program. Dr. Ward is the Computational Science and Engineering lead, and Paul Adams is the Scientific Visualization Center lead.

## ***ERDC Team Members Judge a Local Elementary School Reading Fair***



*Reading Fair entries are viewed by students*

Ginny Miller, ERDC MSRC, Julia Baker, ERDC GSL, and Maggie Sabol, ERDC CHL, participated on January 13, 2004, as Reading Fair judges at Sherman Avenue Elementary School in Vicksburg, Mississippi. After reviewing 125 entries from grades 1-4, judges selected 20 winners, including five first-place finishers. Judges rated the projects based on clarity of writing, creativity, quality, thoroughness, and interest evoked. Winners will go on to compete in Reading Fairs at the district, regional, and state levels.

# Shaping the future

## High School Students Learn About the ERDC MSRC During Career Day Activities

By Ginny Miller

During Career Day activities, local high school students learned that the ERDC MSRC is about more than supercomputers. The high performance computing (HPC) center is home to a variety of careers, from scientific visualization and customer assistance to technical writing and Web design.

“There are many career opportunities in the field of high performance computing,” said Jeanie McDonald, who organized the ERDC MSRC’s participation in the Career Day events at St. Aloysius High School in February and at Vicksburg High School and Warren Central High School in October.

Career Day participation is just one education initiative at the ERDC MSRC, whose leadership realizes the responsibility of training tomorrow’s workforce. “One of our missions is to attract our best and brightest students to science and engineering,” ERDC MSRC Director John West said. “Retaining them,” he added, “will ensure technological leadership for the next generation.”

During the 2003-04 Career Day activities, ERDC MSRC employees not only spoke to students in grades 9-12 about career opportunities but also encouraged them to attend college and to make smart decisions.

The ERDC MSRC also participates in job shadowing programs, tours, and internships.



Technology Transfer Specialist Rose Dykes speaks to students during Career Day activities at St. Aloysius High School



Video Production Specialist David Longmire speaks to St. Aloysius High School students during Career Day

# Shaping the future . . .



*Avis Phillips speaks to Warren Central High School students during Career Day activities*

*Jeanie McDonald addresses students at Warren Central High School during Career Day activities*



*Richard Walters of the ERDC MSRC Scientific Visualization Center demonstrates the SVC's capabilities to a group of Vicksburg High School students*

## *New Commander of ERDC Visits the MSRC*

By Rose J. Dykes

COL James R. Rowan visited the MSRC on March 18. His interest in high performance computing (HPC) and scientific visualization was apparent as he asked questions and commented on the state-of-the-art infrastructure and technology that he observed.

“Ensuring that the U.S. warfighter has the advantage on the battlefield with the help of high performance computing is very important to me, the Corps of Engineers, the Army, and the DoD. The ERDC MSRC plays a major role in helping provide this advantage,” said COL Rowan.

Immediately after COL Rowan assumed command of ERDC on July 26, 2003, he was deployed to Iraq on a 6-month assignment as the deputy theater engineer for Combined Joint Task Force Seven. He officially assumed command of ERDC on March 10, 2004.

“I am thrilled to have the opportunity to serve as the ERDC commander. This assignment is different from any other I’ve had to date. I requested this assignment...I have been an ERDC customer for many years, reaching back for solutions on airfield construction, well-drilling, bridging, snow and ice clearing, river modeling, and communications from Germany, Bosnia, Albania, and, most recently, Iraq. This is my first opportunity to serve with the Corps and my first chance to be part of a research organization,” Rowan



*ITL Deputy Director, Dr. Deborah Dent (far left), and ITL Director, Dr. Jeffery Holland (far right), have just presented an ITL overview to COL James Rowan (center) before he tours the ERDC MSRC HPC and Scientific Visualization centers*

said. All of COL Rowan’s previous assignments have been with active duty military units, and he has been an engineer officer for 25 years.

A West Point graduate, COL Rowan earned two master’s degrees—one in Operations Research and Systems Analysis from the Georgia Institute of Technology and one in Military Arts and Science from the Army Command and General Staff College. He also received a degree from the U.S. Army War College.



*David Stinson, ERDC MSRC, explains the relationship of the ERDC MSRC to the DoD High Performance Computing Modernization Program to COL Rowan as Drs. Dent and Robert Maier, ERDC MSRC, stand by*



*Paul Adams (second from left), Scientific Visualization lead, explains to COL Rowan how the data from the high performance computers are visualized in a context that will help to ensure a better understanding of a project. Looking on in the background (left to right) are Tommy Biddlecome and Richard Walters, Scientific Visualization Center, and David Stinson*

# announcements .....

## ***RSS: A New Way of Communicating with the ERDC MSRC***

*By Ginny Miller*

The ERDC MSRC launched an ambitious project in January to improve the way it communicates with users. Really Simple Syndication, or RSS, is a method of distributing headlines and other Web content in an XML format. The ERDC MSRC is the first in the HPCMP to implement the user-friendly technology.

“We’re doing this for our users,” said John West, ERDC MSRC Director. “This is a new format for reaching out and communicating with people.”

Users may subscribe to any or all of the ERDC MSRC channels by supplying the URLs of the RSS newsfeeds they want to receive through an RSS reader. When a channel has been added, the reader then does all the work, searching for chosen RSS sites – at a frequency determined by the user – and automatically alerting users when new content is available.

“This is a simple way to push information to the users on their own terms,” West said. Prior to RSS, the ERDC MSRC Customer Assistance Center notified its nearly 1,000 users of system outages, platform avail-

ability, holiday schedules, and other ERDC MSRC events exclusively through e-mail. Believing the barrage of “user messages” could be replaced with something better, West suggested RSS as a new method of supplying data to users.

The project was first tested by staff last fall and made available to users at the beginning of the year.

The ERDC MSRC currently provides five RSS newsfeeds for users. The General Interest channel conveys a broad range of news and announcements about the Center, while four system-specific channels provide updates about system problems and events affecting the Cray X1, Cray T3E, the SGI Origins, and Compaq SCs. News is posted as it happens, from once a week to several times a day.

For more information about RSS, visit the ERDC MSRC Web site at [www.erdcmil.com](http://www.erdcmil.com), or contact the ERDC MSRC Customer Assistance Center at 1-800-500-4722 or [msrchelp@erdcmil.com](mailto:msrchelp@erdcmil.com).

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to communicate.



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## *National Geographic Film Crew Shoots Footage at the ERDC MSRC*

By Rose J. Dykes

The production company producing a show for National Geographic on the Murrah Building bombing in Oklahoma City filmed at ERDC on January 30. This show that will be Part 3 of a 12-Part series on forensic engineering. Because of the computing done here, the MSRC was one of the sites chosen for filming at ERDC.

Dr. Paul Mlakar, ERDC Geotechnical and Structures Laboratory (GSL), was the on-camera spokesperson for the ERDC filming. The advanced research capabilities and force protection technologies of the Corps of Engineers was demonstrated with the filming of animations of high performance computing simulations relating to blasts and structures. This was filmed in the MSRC Scientific Visualization Center. Footage was shot in the MSRC High Performance Computing Center as Dr. Mlakar discussed the capabilities of the supercomputers.

Part 3 of the 12-Part series of the documentary, the filming at ERDC, will air in late 2004 or early 2005.



*National Geographic filming crew arrives at the Information Technology Laboratory*



*Dr. Mlakar waits for the camera to roll before he discusses the visualization on the Immersadesk*



*(Left to right) Wayne Stroupe, ERDC Public Affairs Office, quizzes two of the crew members about their equipment as Dr. Paul Mlakar, ERDC GSL, and John E. West, ERDC MSRC Director, watch outside the ERDC MSRC Scientific Visualization Center (SVC)*



*(Left to right) John West, Wayne Stroupe, and the film crew producer discuss the footage to be filmed in the HPC Center*



*John West talks about the fine points of the visualizations with Dr. Mlakar as the crew sets up in the SVC*

## ***ERDC MSRC Conducts a New User Workshop***

The ERDC MSRC hosted a new user workshop organized by Dean Hampton for new users on April 20, 2004. Bill Renaud presented an overview of the ERDC HPC machines. He discussed other topics such as obtaining accounts, the Load Sharing Facility (LSF) scheduler system, disk space management, using authentication software, how to write and submit scripts to run jobs, using the mass storage system, and the utilities available.



*Bill Renaud making his presentations*



*New users (seated) and Dr. Ruth Cheng and Bobby Hunter (standing left to right), ERDC MSRC*

Bobby Hunter and Dr. Ruth Cheng packaged the parallel WASH123D software, demonstrated parallel job submission/launches, and showed the EasyHPC system (see page 17). The purpose of this workshop was to aid in the migration to ERDC HPC machines, promote the parallel WASH123D code to a production stage, and support users for the Philadelphia District's technical project.



## ***ERDC Researcher Named to the User Advocacy Group***

Dr. Stephen Ketcham, ERDC Cold Regions Research and Engineering Laboratory, was named in March as a member of the User Advocacy Group (UAG) for users of the DoD HPCMP. The group's purpose is to influence policies and practices of the program, to facilitate the exchange of information between the user community and the HPCMP, to serve as an advocacy group for all HPCMP users, and to advise the DoD HPCMP Office on policy and operational matters related to the HPCMP. Membership consists of four members from each Service and one member representing participating DoD agencies. As a member of the UAG, Dr. Ketcham will ensure that the needs of ERDC users of the HPCMP resources will be identified and met. (Taken from the April 30th ERDC Rollup)

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](mailto:msrchelp@erdc.hpc.mil)



*Edward J. Welch (front, second from left), Chief of Police, New York City Police Department, with Paul Franco, U.S. Army Engineer District, New York (front, far left), Marc Ryan, General Dynamics Corporation (behind Edward Welch), Dr. Jeffery Holland (to right of Edward Welch), ERDC ITL Director, Dr. Bob Welch (second from right), ERDC ITL, and John E. West (far right), ERDC MSRC Director, April 22, 2004*



*(Front row) The Honorable John Paul Woodley, Jr., Assistant Secretary of the Army, Civil Works (center), with Dr. Jeffery Holland (far left) and John West (far right). (Back row, left to right) COL James R. Rowan, ERDC Commander, Dr. Dave Pittman, GSL Acting Director, and Dr. James Houston, ERDC Director, April 22, 2004*





*John West (foreground) talks with (left to right) Dr. Jimmy Johnston, U.S. Geological Survey; Dr. John H. Marburger, Science Advisor to President George W. Bush, and serves as Director of the White House Office of Science and Technology Policy; Dr. Houston; COL Rowan; and Dr. Gene Whitney, National Science and Technology Council. Dr. Charles G. Groat (back, center), Director, U.S. Geological Survey was also with the group, March 24, 2004*



*(Left to right) Don Wilson, Navigation Branch Chief, ERDC CHL, and from the Portland District, Bob Buchholz, Hydraulic Design Section Chief; Ron Mason, Hydraulics and Hydrology Branch Chief; Mike Ott and Laurie Rice, Engineers in Training, Engineering and Construction Division; and LTC Charles Markham, Deputy District Engineer/Acting District Engineer, March 17, 2004*



*David Stinson (far right), ERDC MSRC, with Mid-West Natural Resources Group Spring Meeting attendees, March 2, 2004*

*(Left to right) Mr. Andy Bruzewicz, Office of Homeland Security; Ed Hecker, Chief, Office of Homeland Security; Dr. Reed Mosher, ERDC GSL; John Meador, Deputy Chief, Infrastructure Support Branch, Office of Homeland Security; Dr. Cary Butler, ITL Technical Director; Dr. Bob Welch, ITL; and Bob Athow, ERDC MSRC, January 22, 2004*



*(Standing) John West talks with Dr. Dixon Butler, Committee on Appropriations, U.S. House of Representatives (seated at table); Drs. Holland and Houston (seated behind Dr. Butler); and Miguel Valenciano, ERDC MSRC Scientific Visualization Center, January 6, 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.

AHPCRC	Army High Performance Computing Research Center	ITL	Information Technology Laboratory
API	Application Programming Interface	LES	Large-Eddy Simulation
BB	Big Brother	LSF	Load Sharing Facility
CFD	Computational Fluid Dynamics	MPI	Message Passing Interface
CHL	Coastal and Hydraulics Laboratory	MSP	Multistreaming Processor
CPU	Central Processing Unit	MSRC	Major Shared Resource Center
CRREL	Cold Regions Research and Engineering Laboratory	NJDEP	New Jersey Department of Environmental Protection
CSM	Computational Structural Mechanics	NPS	Naval Postgraduate School
DMT	Deformation Mapping Technique	PBS	Portable Batch System
DNS	Direct Numerical Simulation	PE	Processing Element
DoD	Department of Defense	PET	Programming Environment and Training
DOE	Department of Energy	PIPS	Polar Ice Prediction System
ERDC	Engineer Research and Development Center	RSS	Really Simple Syndication
FNMOCC	Fleet Numerical Meteorology and Oceanography Center	SIAM	Society for Industrial and Applied Mathematics
GMS	Groundwater Modeling System	SMS	Surface-Water Modeling System
GMV	General Mesh Viewer	SSP	Single-Streaming Processor
GSL	Geotechnical and Structures Laboratory	SVC	Scientific Visualization Center
HPC	High Performance Computing	TCE	Trichloroethylene
HPCMP	High Performance Computing Modernization Program	UAG	User Advocacy Group
		USEPA	U.S. Environmental Protection Agency

## training schedule .....

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

<https://okc.erd.c.hpc.mil>

Questions and comments may be directed to PET training at (601) 634-3131, (601) 634-4024, or [PET-Training@erd.c.usace.army.mil](mailto:PET-Training@erd.c.usace.army.mil)



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