Navigator

NAVO MSRC FALL 2008

Behind the Curtain

An opportunity for NAVO MSRC senior staff to reflect on the NAVO MSRC's past, present, and future endeavors.

In Other Words...

Christine Cuicchi
Computational Science and Applications Lead,
NAVO MSRC

"When fortune comes, seize her firmly by the forelock, for, I tell you, she is bald at the back."

- Leonardo Da Vinci

When the NAVO MSRC found itself with a two-thirds empty machine room floor after the IBM P4 system MARCELLUS was removed, Director Tom Dunn seized the opportunity to kick off a number of facility upgrades in anticipation of the demands that new High Performance Computing (HPC) systems would place on the Center's infrastructure. Dave Cole, Acting Associate Director (Plans and Programs), details these upgrades on page 5—along with a long-anticipated update on the dogs that accompanied him and his wife, Leona, as they evacuated from Hurricane Katrina in 2005. The facility upgrades, overseen by Jennifer Rabert and later, new government staff member Rob Thornhill of the NAVO MSRC, were begun and completed in 2008 in time for the arrival of our two new HPC systems, DAVINCI (IBM P6) and EINSTEIN (Cray XT5), and our new mass storage server, NEWTON (Sun M5000).

"The most incomprehensible thing about the world is that it is at all comprehensible."

- Albert Einstein

The computing power that these new systems bring will make the NAVO MSRC the most powerful in the Department of Defense High Performance Computing Modernization Program—for the time being. It is a function of the industry that those on top are never on top for long; we continue to lean on our IBM P5+ workhorses BABBAGE and PASCAL while diversifying and vastly increasing the scientific computing capabilities we provide to our users with our new arrivals. Four Capability Application Projects (CAP) will run on both DAVINCI and EINSTEIN, providing researchers with the capability of running jobs of up to 4,256 and 12,736 cores in size, respectively. We continue to take pride in our role in nurturing terascale scientific research and engineering in support of the warfighter.

"If I have seen further, it is by standing on the shoulders of giants."

- Isaac Newton

Onsite expertise and data storage: these two elements provide the critical foundation for the computational science accomplished on our systems. Although it has received decidedly less press than our incoming HPC systems, our new Sun M5000 archive server NEWTON will provide even more stability and faster data archive access to support the data storage demands, which are expected to double as EINSTEIN and DAVINCI are brought online. We have also strengthened the backbone of our Remote Storage Facility infrastructure, as detailed on page 9. Over the past six months we have increased our original government staff of seven to eleven, strengthening our technical and facilities expertise; please take an opportunity to meet our newest team members starting on page 14.

It has been, and continues to be, our pleasure to adapt, expand, and advance to serve the needs of our user community.

The Naval Oceanographic Office (NAVO) Major Shared Resource Center (MSRC): Delivering Science to the Warfighter

The NAVO MSRC provides Department of Defense (DoD) scientists and engineers with high performance computing (HPC) resources, including leading edge computational systems, large-scale data storage and archiving, scientific visualization resources and training, and expertise in specific computational technology areas (CTAs). These CTAs include Computational Fluid Dynamics (CFD), Climate/Weather/Ocean Modeling and Simulation (CWO), Environmental Quality Modeling and Simulation (EQM), Computational Electromagnetic and Acoustics (CEA), and Signal/Image Processing (SIP).

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Five Dogs, a Hurricane, and Two IBM Power5+s – a Third Year Update

Dave Cole, NAVO MSRC

NAVO MSRC Expands Again

Located at Stennis Space Center (SSC) in Mississippi, the NAVO MSRC maintains and provides premier High Performance Computing (HPC) capability with primary emphases on support of the largest, most computationally intensive HPC applications and delivery of time-critical HPC services to directly support Department of Defense operations worldwide. The large scale, power hungry HPC systems used to satisfy the computational requirements place extraordinary demands on Center infrastructure.

After installation of the Technical Insertion 2004 (TI-04) systems, the building hosting HPC systems for the NAVO MSRC lacked sufficient space, power, and cooling capabilities to support installation of additional supercomputers.

In anticipation of future support requirements, our former Director Steve Adamec developed an innovative plan to renovate a steel reinforced concrete building that had been in mothball status for more than a decade at the Army Ammunition Plant complex located at the SSC.

Implementation of the plan had just begun when Hurricane Katrina struck the Mississippi Gulf Coast on 29 August 2005. The facility easily withstood the battering hurricane force winds including the newly installed metal roof rated for sustained wind speeds up to 150 miles per hour.

Three years ago, the Spring 2006 edition of the Navigator included an article that gave an account of my evacuation from the Mississippi Gulf Coast prior to landfall of Hurricane Katrina, a brief description of the journey home, and my eventual return to work at the NAVO MSRC.

The intent of the article was to provide a personalized Katrina account to provide insight into the many challenges faced by members of the NAVO MSRC community. It also told the story of the rescue of two beagles from a local kennel for a friend who was out of the country and their addition to our "pack" of terriers – an addition that brought the pet evacuation count to five small frisky dogs.

This article serves as a sequel to let the members of the High Performance Computing Modernization Program (HPCMP) community know about our recovery and to briefly describe the results of significant facilities infrastructure modifications — modifications that were accomplished at a time when many NAVO MSRC members were rebuilding their homes and their lives. Oh yes, it also includes an update of how the five small frisky dogs have fared.

Renovation work at the new facility (See box, this page) resumed three weeks after the Gulf Coast and the NAVO MSRC began recovery efforts and was completed in time to support installation of the IBM P5+ systems BABBAGE and PASCAL.

The new facility provided approximately 11,000 square feet of 30-inch raised floor space with approximately 800 tons of cooling capacity, and a 1000 Kilowatt (KW) Uninterruptible Power System (UPS) for conditioned power. With the

Continued Next Page...

NAVO MSRC space containing BABBAGE and DAVINCI.

addition of a second 1000 KW UPS to support the installation of the Technical Insertion for Fiscal Year 2008 (TI-08) IBM P6 DAVINCI, 2000 KW of conditioned and backup generator power are now available for High Performance Computing (HPC) systems support.

With the decommissioning and removal of the IBM P4+ MARCELLUS system in January 2007 from the original NAVO facility, MSRC Director Tom Dunn recognized this as a unique opportunity to renovate our aging facilities infrastructure.

Renovation requirements were presented to the High Performance Computing Modernization Office (HPCMPO) in December 2007 and were subsequently approved for implementation. Upgrades to the original MSRC facility include:

- Removal of unused power whips and cables under the raised floor and replacement of floor water detector tapes.
- Replacement of the above floor fire suppression system with overhead FM200 and removal of an existing water based system.
- Replacement of the raised floor that includes tiles rated at 2000 pounds per square inch.
- Installation of four 60-ton computer room units and modification of the false ceiling to provide sufficient cooling and air flow to accommodate large scale HPC systems.

Completed in time for the delivery of the Cray XT5 Einstein in September, the renovated space offers approximately 7500 square feet of 18-inch raised floor space with 800 tons of cooling capacity, 1000 KW of conditioned power, and 1750 KW of backup generator power for HPC systems support.

As described in the closing paragraph of the Spring 2006 edition of the Navigator, Hurricane Katrina severely impacted the lives of the members of the MSRC. Thirty percent of the MSRC team suffered catastrophic damage to their homes, rendering the home uninhabitable or totally devastated.

The transformation of a building in mothball status at the Army Ammunition Complex into a world-class HPC support facility at a time when many team members were rebuilding their homes and their lives demonstrates their commitment to the HPCMP community.

The recent renovation of the original MSRC facility further demonstrates the NAVO MSRC support of the HPCMP mission to accelerate the development of advanced defense technologies for the warfighter via supercomputing.

And last, but not least, the long-awaited update on the five small dogs: during the evacuation they experienced a sense of displacement and anxiety that was further deepened by their brief stay at a “two star” dog kennel in my hometown of Minden, LA.

Reunited with their owner, the two beagles have fully recovered and start each morning by waking up the neighborhood. The three “terrible” terriers are thrilled with their new home, which came with a big backyard enclosed by a privacy fence. In short, the five small dogs are as frisky as ever.

Five frisky dogs - two singing beagles and three "terrible terriers" - taking it easy.

Advance Reservations: Back on Babbage and Better than Ever

Christine Cuicchi, Computational Science and Applications Lead

Want it all, and want it now? We can't give you the whole system on demand, but we can give you up to 256 processors with an advance reservation on the P5+ system, BABBAGE. The Advance Reservation System (ARS), which was available on KRAKEN, has been moved to BABBAGE for Fiscal Year 2009 and is available to any user with BABBAGE allocation.

As with the previous capability on KRAKEN, users may request a specific available run time to run interactive jobs, real-time simulations, or batch jobs. Users will authenticate to the front end of the ARS portal (link available at http://www.navo.hpc.mil) via Kerberos (Figure 1). First-time users will be directed to request an account on the online reservation portal of the ARS. This account is not related to allocated accounts on the High Performance Computing (HPC) systems.

After establishing an online reservation portal account and logging in to the portal screen as shown in Figure 2, a user will be able to see how many processors are available for reservation on any given day in the calendar view. By simply clicking on the day being targeted for reservation, a user will see an hour-by-hour list of available processor counts (Figure 3).

Users may request--via drop-down menus--a number of processors (up to 256, divisible by 16 processors per node) for a user-specified amount of time of up to 48 hours, delineated in one-hour increments. Users will also be able to specify, via a drop-down menu, the project to which the reservation hours will be charged. In the example shown in Figures 4 and 5, a request is being made for 48 processors (4 nodes) for 4 hours on 10 October 2008, starting at 1700 Greenwich Mean Time (GMT).

Checking the available hours for 10 October via the calendar now shows that there are 48 fewer processors available during the time period for

Continued Next Page...

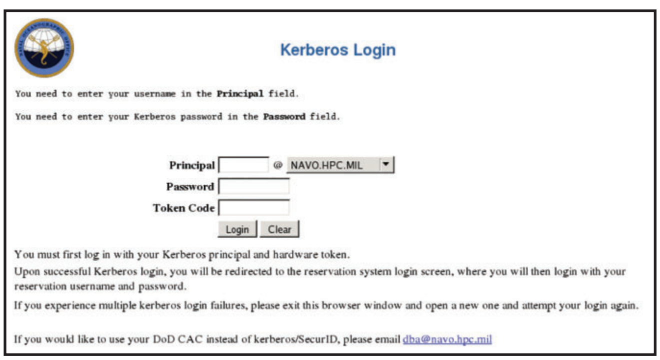
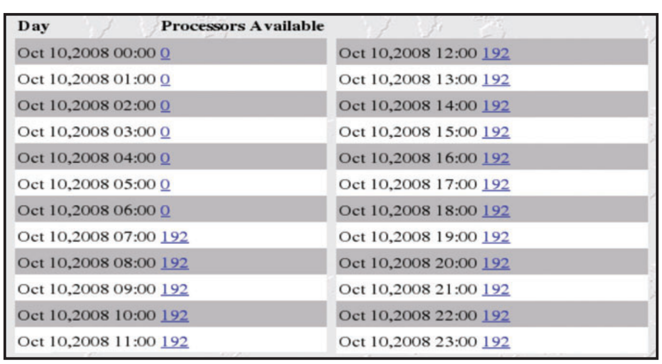


Figure 1. ARS Kerberos login.

Figure 2. ARS Portal login screen.



Day	Processors Available		
Oct 10,2008 00:00	0	Oct 10,2008 12:00	192
Oct 10,2008 01:00	0	Oct 10,2008 13:00	192
Oct 10,2008 02:00	0	Oct 10,2008 14:00	192
Oct 10,2008 03:00	0	Oct 10,2008 15:00	192
Oct 10,2008 04:00	0	Oct 10,2008 16:00	192
Oct 10,2008 05:00	0	Oct 10,2008 17:00	192
Oct 10,2008 06:00	0	Oct 10,2008 18:00	192
Oct 10,2008 07:00	192	Oct 10,2008 19:00	192
Oct 10,2008 08:00	192	Oct 10,2008 20:00	192
Oct 10,2008 09:00	192	Oct 10,2008 21:00	192
Oct 10,2008 10:00	192	Oct 10,2008 22:00	192
Oct 10,2008 11:00	192	Oct 10,2008 23:00	192

Figure 3. Hour-by-hour list of available processors.

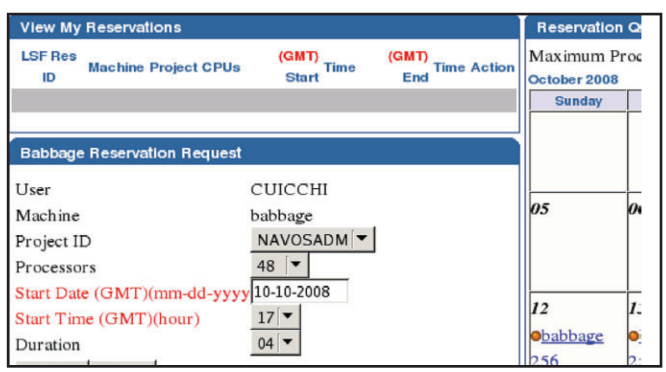


Figure 4. Selecting reservation options.

which the reservation was requested (See Figure 6).

Once the reservation request is made, the user will receive an email containing a list of the specific nodes reserved as well as the Load Sharing Facility (LSF) reservation identification number (reservation_id) to be used in submitting jobs to the reserved nodes. This reservation identification number must be used to submit batch jobs in the following manner:

```
bsub -U reservation_id ... < script
```

Users who wish to run interactive jobs should submit them at the beginning of the reservation. Running the showq command on BABBAGE will allow users to see a list of reservations as well, as illustrated in Code 1.

A user can also check the status of a reservation at the ARS portal as shown in Figure 7.

All reservations will begin at the start time the user has requested. After receiving the confirmation email, users will have the ability to cancel their reservations up to 30 minutes prior to the reservation start time (See Figure 7).

It is important to note that if the reservation is not cancelled, system utilization will be charged for these nodes regardless of how, or if, the nodes are used.

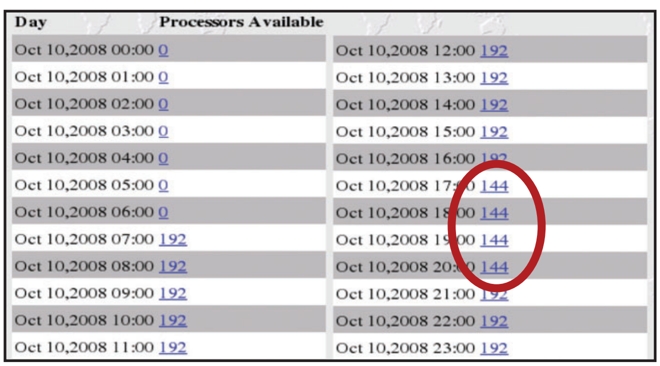
In its previous incarnation, the ARS ran on dedicated nodes, which ensured that the nodes were available to users for advance reservation at all times. In the spring of 2008, the NAVO MSRC added a backfill capability to ARS so that the nodes earmarked for advance reservation would still be available to regular batch queues when demand for advance reservations waned.

Users planning advance reservation requests should take into account that some, or all, of these nodes may be backfilled for up to 48 hours from the present time. Again, node availability by the hour can be found by clicking on the calendar day in which the user is interested in placing a reservation.

The NAVO MSRC will be a leading site in reproducing this advance reservation capability under the Portable Batch System (PBS) Pro workload management system. Future plans call for the possible development of a single ARS portal that would handle advance reservation requests on a number of HPC systems across the Department of Defense HPC Modernization Program.

For more information about the ARS and access to the ARS portal, please visit: http://www.navo.hpc.mil.

Figure 5. Notification of successful reservation request.



Day	Processors Available
Oct 10,2008 00:00 0	Oct 10,2008 12:00 192
Oct 10,2008 01:00 0	Oct 10,2008 13:00 192
Oct 10,2008 02:00 0	Oct 10,2008 14:00 192
Oct 10,2008 03:00 0	Oct 10,2008 15:00 192
Oct 10,2008 04:00 0	Oct 10,2008 16:00 192
Oct 10,2008 05:00 0	Oct 10,2008 17:00 144
Oct 10,2008 06:00 0	Oct 10,2008 18:00 144
Oct 10,2008 07:00 192	Oct 10,2008 19:00 144
Oct 10,2008 08:00 192	Oct 10,2008 20:00 144
Oct 10,2008 09:00 192	Oct 10,2008 21:00 192
Oct 10,2008 10:00 192	Oct 10,2008 22:00 192
Oct 10,2008 11:00 192	Oct 10,2008 23:00 192

Figure 6. Reduction of available cores due to requested reservation.

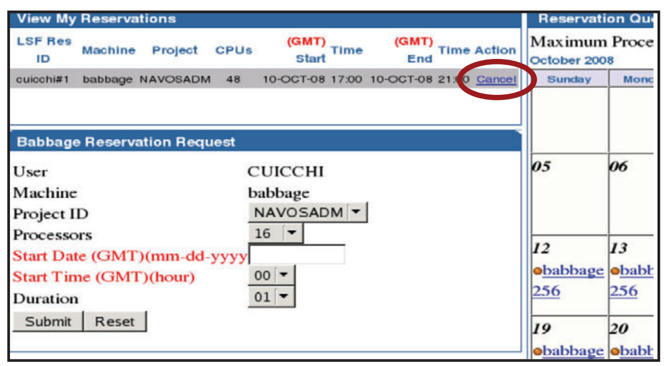


Figure 7. Reservation status and cancel option.

```
b5n1...cuicchi> showq
ADVANCED RESERVATIONS----------
RESV ID                  PROC              RESERVATION WINDOW
res# 1 :   time1=1223658000   time2=1223672400
cuicchi#1                48                Fri Oct 10 17:00:00 2008 - Fri Oct 10 21:00:00 2008
```

Code 1. Advance reservations as they appear in showq command output.

Quarterly Tests Reveal Exceptional Performance Stability for IBM Platforms at NAVO MSRC

Christine Cuicchi, Computational Science and Applications Lead, NAVO MSRC

Dr. Paul Bennett, Computational Science and Engineering (CS&E) Group, Engineer Research Development Center (ERDC) MSRC

Sustained system performance—it's something most users expect of the well-developed high performance computing (HPC) systems—and the IBM P4+ and P5+ platforms at NAVO MSRC have demonstrated excellent sustained performance over the past several years.

Every three months, Dr. Paul Bennett of the ERDC MSRC CS&E group runs a Sustained System Performance (SSP) test on Department of Defense (DoD) High Performance Computing Modernization Program (HPCMP) systems to evaluate and compare the systems' performance over their time in service to the Program.

The test, modeled after the National Energy Research Scientific Computing (NERSC) Center's SSP test[1], consists of a number of application codes and input data sets that represent a composite of the HPCMP's systems workload. Each application is run on both "standard" and "large" size data sets, and the full suite as characterized by Dr. Bennett will, "stress the processing elements, main memory, and file I/O systems to determine the existence of compiler optimization issues, issues with communication libraries, problems with I/O subsystems, problems with libraries that have been recompiled in a different way, software or hardware issues specific to the interconnect, changes to the runtime environment, or the application of security patches that adversely affect performance."

Figures 1 and 2 show the sustained system performance of KRAKEN (IBM P4+) and BABBAGE (IBM P5+) per application code over their lifetimes. System performance for both systems is presented as relative to the system's original Technology Insertion (TI) benchmarked application performance in TI-04 and TI-06, respectively. The SSP tests reveal that KRAKEN's relative performance increased over its time in service while remaining fairly stable over its last year of life and that BABBAGE's relative performance has been extremely stable with a slight increase in performance for a number of application codes. These SSP tests will also be run on DAVINCI and EINSTEIN once the two new systems enter their allocated phases at NAVO MSRC.

Figure 1

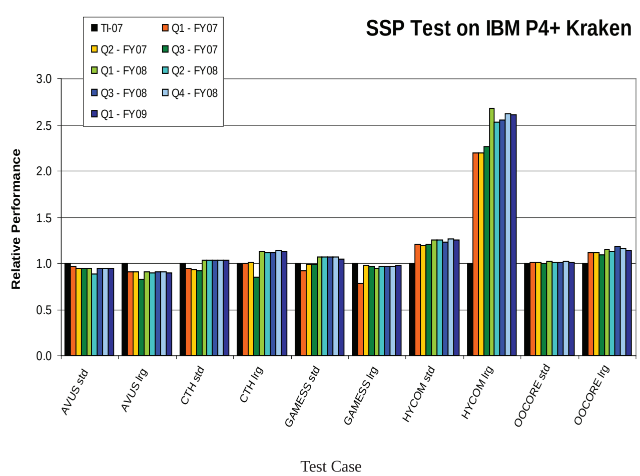
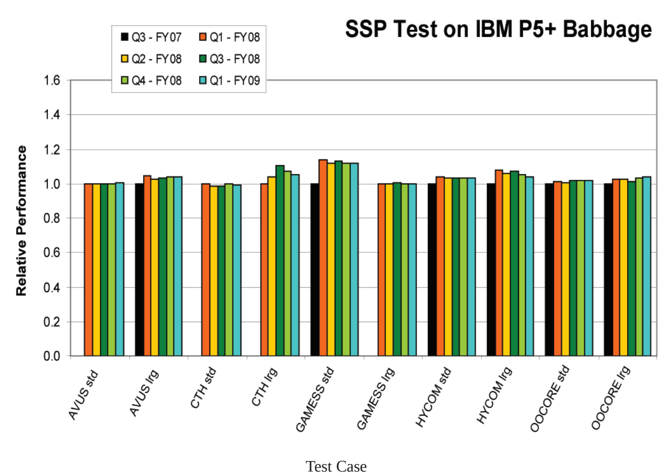


Figure 2



1. W. Kramer, J. Shalf, E. Strohmaier, "The NERSC Sustained System Performance (SSP) Metric," Paper LBNL-58868, Lawrence Berkeley National Laboratory, 2005.

DAVINCI AND EINSTEIN BRING TH

The summer of 2008 has been an eventful one at the NAVO MSRC. Two major happenings were the installations of both the Cray XT5 EINSTEIN and the IBM P6 DAVINCI. With the completion of these installations and the decommissioning of our venerable IBM P4s (KRAKEN and ROMULUS), the total computing capacity at NAVO has quadrupled to 233 Teraflops (TFLOP).

To kick off this summer's festivities, the NAVO MSRC received DAVINCI, an 80 TFLOP IBM Power6 system packing 4,256 4.7 Gigahertz (GHz) compute cores. It also contains 10 Terabytes (TB) of main memory and 437 TB of disk space.

Another amazing feature of DAVINCI is that it is completely water-cooled – what IBM terms a "hydro-cluster." Water is piped into the system and runs across the processors via copper plating to dissipate their heat. DAVINCI is also different in that each of its 14 cabinets has a door that passively removes heat (known as a heat-exchanger door). These doors also utilize water to reduce the amount of heat allowed to enter the computer room facility.

According to IBM, a hydro-cluster system similar in size to DAVINCI needs roughly 80 percent less air conditioning than a traditional air cooled system. Total energy consumption should also be reduced by around 40 percent. These savings allow the NAVO MSRC to move towards becoming a more "green friendly" facility. Though the IBM Power series systems have been a mainstay at the NAVO MSRC for years, the DAVINCI system will prove to be a worthy successor.

DAVINCI

With the installation of DAVINCI and EINSTEIN, the NAVO MS computing technology available, with the best support poss

. . . AND THE BU

heir Computing Power to NAVO MSRC

The installation of the Cray XT5 EINSTEIN will forever be remembered as "the one that finally happened." As production of the system completed, Cray prepared to ship the system, and anticipation at the NAVO MSRC was on the rise. Little did we know that Mother Nature had other plans.

Initially, the system was to be delivered the week after Labor Day, but along came Hurricane Gustav to nix those plans. The shipment was delayed. As time drew near for the next attempt, Hurricane Ike decided to make his way into the Gulf of Mexico, bringing yet another delay in the shipment date. The system finally made its way to the MSRC in mid-September, but only after breaking the record for most hurricanes (two) to delay an installation. The previous record of one delay was held by the SAPPHIRE system at the U.S. Army Engineer Research and Development Center (ERDC) MSRC for its bout with Hurricane Katrina in 2005.

While already a record holder, EINSTEIN is also the largest in the Department of Defense in peak performance (117 TFLOP), number of cores (12,856), total available main memory (25 TB), and disk space (518 TB). It recently recorded a LINPACK number of 93 TFLOP. Another interesting EINSTEIN factoid is that it is one of a select number of Cray XT systems to have a vinyl skin applied to its exterior. The skinning of the new XT systems has become so popular that Cray now has a laminating press to apply it. The previous XT3 generation had a textured door that would not allow for an overlay. In response to the ERDC MSRC desire for its new XT4 system JADE to have camouflaged doors, Cray developed smoother cabinet doors to allow the skin to be applied. So, EINSTEIN, already an amazing system, looks good too. - Bryan Comstock, NAVO MSRC, Computer Scientist

Einstein

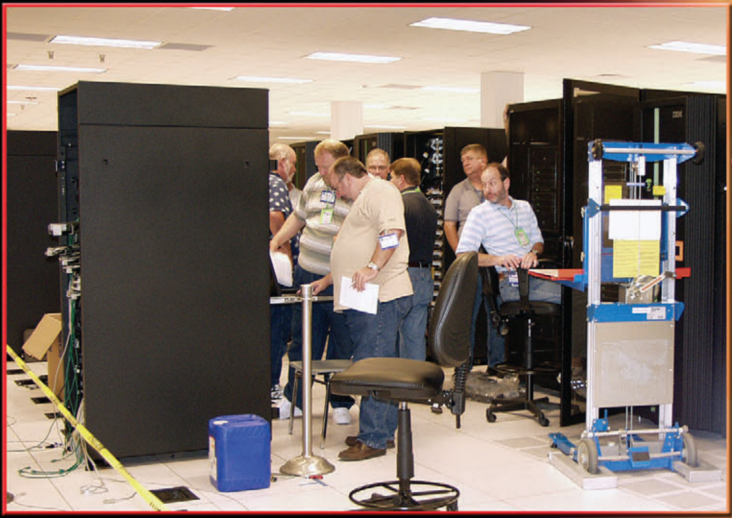
RC continues its mission to provide the best high performance
sible, to the military and academic research communities.

LD GOES ON . . .

The Porthole

DoD HPCMPO, IBM, and Government Oversight representatives participate in the TI-08 Capabilities Test for the new IBM Power6 HPC system DAVINCI.

CRAY XT5 EINSTEIN installation team.



IBM P6 DAVINCI installation team.

Teachers with the Mississippi State University-sponsored Industry-Education Partnerships Workshop view a briefing on the field of high performance computing and its role at the NAVO MSRC.

Casey Bretti (AFRL) and Sheila Carbonette (NAVO) participate in the Enhanced USER Experience team meeting at AFRL.

Lockheed Martin Database Administration Process Improvement Group gathered at NAVO September 23-25.

Welcome Aboard! NAVO MSRC Welcomes

Tom Brown

Tom Brown arrived in September to be the Associate Director for Operations at the NAVO MSRC and the National Center for Information Processing and Storage (NCCIPS) data center at the Stennis Space Center, Mississippi. Tom comes to the MSRC and NCCIPS from Arnold Engineering Development Center, Tennessee, where he served in numerous leadership positions. Prior to his move to Stennis, he served as part of the Office of Secretary for Defense High Performance Computing Modernization Program Office (HPCMPO) senior staff as Deputy Centers Program Manager with responsibilities for managing and delivering services to all the DoD HPC MSRCs. "Over the years I've been fortunate to work with many of the great folks at NAVO as a colleague in the larger HPC community; now I'm proud to now be part of the Stennis team," said Tom.

Starting with the Department of the Air Force as a student aide, Tom has served in numerous Information Technology (IT) positions during his 30+ years of government service. His experience includes assignments at three Air Force bases with three different Major Commands (MAJCOMS) on Center and Headquarters MAJCOM staffs, and as senior member of the HPCMPO staff.

As a seasoned IT professional, Tom brings the NAVO MSRC and NCCIPS extensive knowledge of corporate leadership of Information Resource Management (IRM) programs and staff, communications, and computer systems planning and management.

He is also using his experience in IT acquisition, business/engineering computer and communications architectures, modeling and simulation systems design, software engineering, IT integration and program management, computer security, and telecommunications systems management to improve the MSRC and NCCIPS. He holds two masters degrees, and his executive training and experience includes the Defense Leadership and Management Program (December 2004 graduate) and Chief Information Officer Certification from the National Defense University.

Rob Thornhill

Rob Thornhill is a native Mississippian who is the new NAVO MSRC Facilities Engineer. As such, he oversees all facilities planning, maintenance, and upgrades. With the recent renovation of the original MSRC space and the new facility and the installation of EINSTEIN and DAVINCI, Rob has been very, very busy. (See Five Dogs, a Hurricane, and Two IBM Power5+s – a Third Year Update on page 5 and DAVINCI and EINSTEIN Bring Their Computing Power to NAVO MSRC, page 10).

Though Rob is not new to the Naval Oceanographic Office (NAVOCEANO) (he started as a contractor in 2003 and joined the Government ranks in 2006), it wasn't until this spring that he joined the NAVO MSRC team.

Along the way from the University of Southern Mississippi to the NAVO MSRC, Rob took a detour through the aggregate mining industry ("That's a fancy way of saying 'I worked in a gravel pit.'"), where he learned the advantages of indoor work in the summer and winter, as well as maintenance and planning skills. These are skills that he refined and applied to the information technology arena through his prior work with Navy Marine Corps Intranet (NMCI) implementation at NAVOCEANO.

Of his move to the NAVO MSRC from NAVOCEANO, Rob says, "While working with NAVOCEANO, I was presented an opportunity to become part of the MSRC team. I have always been somewhat in awe of the 'the big, fancy computers' and could not pass up the chance to actually become a part of it."

New User Support Team Members

Bryan Comstock

Bryan Comstock is a proud Gulf Coaster who recently joined the NAVO MSRC as the primary Government Point of Contact (POC) for the Consolidated Customer Assistance Center (CCAC), the Consolidated Software Initiative (CSI), the Customer Satisfaction Survey (CUSS) and the Enhanced User Environment (EUE). Taken down to its essence, this means: "I will have an active role in forming, monitoring, and modifying the policies, procedures, and activities that affect our users on a daily basis. As the backup Outreach and Challenge project POC, I assist the primary POC, Christine Cuicchi, in supporting the NAVO operational users and Challenge users. Being a new member of the government staff, I hope to continue to provide a high level of service in these areas."

Bryan started his road to the MSRC at the University of Southern Mississippi, which led to a position at the Mississippi State University's Engineering Research Center. Later, he joined the MSRC as a contractor providing user support analysis, and, after a brief foray as a Software Engineer for Planning Systems, Inc., he returned to the NAVO MSRC as part of its Government management team. One of the best parts of being part of the NAVO MSRC team, he says, is the opportunity to observe and support the various scientific applications being run on the High Performance Computing (HPC) systems.

While he finds them all interesting, the ones relating to weather and mechanics are especially attractive: "Growing up on the Gulf Coast and seeing hurricanes firsthand, I've always had a fascination with weather; the Climate/Weather/Ocean (CWO) Modeling and Simulation Computational Technology Area (CTA) would have to be my favorite. Before going into computer science, I was considering becoming a mechanical engineer, so the Computation Fluid Dynamics (CFD) or Computational Structural Mechanics (CSM) CTAs also interest me."

Morgan Harrison

Morgan Harrison, the newest NAVO MSRC computer scientist, comes to the NAVO MSRC after five years of system administration and user support that the Mississippi State University High Performance Computing Collaboratory (HPC2). Though part of the NAVO MSRC team for only three months (he jokes "I joined so I could say 'I'm from the Government and I'm here to help you.'"), Morgan is quickly integrating into the MSRC user support community and providing valuable technical expertise in systems management and overall MSRC system architectures.

Morgan's new position is, he states, the next logical progression in working with bigger, faster, more interesting High Performance Computing systems. Though he hasn't managed to do this yet at the NAVO MSRC, he says, "My favorite thing to do whenever I get a new computer is to pull the case off and see what the insides look like. When Operations and the System Administrators turn their backs, I might go at DAVINCI or EINSTEIN."

Working at the MSRC is exciting because, Morgan says, "Even though I haven't been part of the NAVO MSRC team long, I feel like I'm already contributing behind the scenes to improve our users' experience."

Navigator Tools and Tips

Using PBS at the NAVO MSRC

Sheila Carbonette, User Support, NAVO MSRC
Morgan Harrison, Computer Scientist, NAVO MSRC
Bryan Comstock, Computer Scientist, NAVO MSRC

The Portable Batch System (PBS) is available on the IBM P6 and CRAY XT systems at the NAVO MSRC. This guide will serve as an overview of PBS and offer a comparison of PBS, Load Sharing Facility (LSF) and LoadLeveler queuing system commands, environment variables, and batch scripts.

In order to use PBS, users do not need to add anything to their startup files. PBS-related environment variables and paths have been added to the IBM and CRAY system files to set up PBS as part of the user login session.

PBS, LSF, and LoadLeveler are alike in that they all are products that schedule user jobs in a batch environment. All three schedulers have commands that allow users to submit jobs, check job and queue status, and hold/cancel jobs. The following tables provide a brief comparison of the commands and utilities of the schedulers as well as list the more common commands.

PBS Script Tips

Writing a PBS script is straightforward. However, a few tips regarding writing PBS scripts are always helpful:

- Do not use PBS environment variables in the #PBS directives.
- Standard output and error can be combined into one file using the "-j oe <filename>" option.
- Omitting the -o and/or -e option(s) sends std output and/or error to a filename in the format of:

  <job name>.[oe]<job id>.

- Omitting a job name results in output and error filenames in the format of:

  <PBS script name>.[oe]<job id>.

Sample PBS Scripts

A PBS script to run a serial job will look something like this:

```
#!/bin/csh
#PBS -N serialjob               # Name of the job.
#PBS -o serialjob.out           # Appends std output to
                                #file serialjob.out.
#PBS -e serialjob.err           # Appends std error to
                                #file serialjob.err.
#PBS -A NAVOSLMA                # Charging Project ID.
#PBS -l walltime=01:30:00       # Wall clock time of
```

Queuing System Command Comparison			
PBS	**LSF**	**LoadLeveler**	**Description**
qsub script	bsub < script	llsubmit script	Submit a job script for execution.
qstat tracejob	bjobs bhist	llq	Show status of running and pending jobs. Displays historical information about your jobs.
qdel	bkill	llcancel	Kill a job.
qhold	bstop	llhold	Hold a job.
qstat -Q qstat -Qf	bqueues	llclass showqlimits	Show configuration of queues.
	busers		Displays information about users and groups.
	bpeek		Displays the stderr and stdout of an unfinished job.
	bacct		Displays accounting information for finished jobs.
	bhosts	llstatus	Summarize load on each host.

NOTE: With PBS "qsub" is used to submit a job while "qstat" can be used to check the status. The job remains in a pending state (PEND) until all resources are available.

Once the resources are available, the job is started by PBS and is now in a running state (RUN). "qstat -Qf" can be used to show the configuration of the queues.

```
                                        #1 hour and 30 min.
#PBS -q standard                        # Queue name.
#PBS -l select=1:ncpus=1                # Number of CPUs.
#
# Compile Fortran code
xlf90 -o serial.exe serial.f
# Run serial executable on 1 cpu of one node
./serial.exe
#End of Sample PBS Script
```

While a PBS script to run a Parallel Message Passing Interface (MPI) job will resemble this:

```
#!/bin/csh
#PBS -N mpijob                          # Name of the job.
#PBS -o mpijob.out # Appends std output to file mpijob.out.
#PBS -e mpijob.err  # Appends std error to file mpijob.err.
#PBS -A NAVOSLMA                        # Charging Project ID.
#PBS -l walltime=02:00:00   # Wall clock time of 2 hours.
#PBS -q standard                        # Queue name.
#PBS -l select=4:ncpus=8:mpiprocs=8     # Request 4
                                        8-processor "chunks"
#PBS -l place=scatter:excl              # Allocate separate
                                        #nodes exclusively
#
# Run an MPI job with the IBM parallel job starter "poe"
poe ./c_hello
#End of Sample PBS Script
```

And a PBS scrip to run a parallel Open MP job will look like this:

```
#!/bin/csh
#PBS -N ompjob                          # Name of the job.
#PBS -o ompjob.out                      # Appends std output to file
                                        #ompjob.out.
#PBS -e ompjob.err                      # Appends std error to
                                        #file ompjob.err.
```

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Job Script Frequently Used Options

PBS	LSF	Loadleveler	Option
#PBS -N jobname	#BSUB -J jobname	#@ job_name = jobname	assigns name to job
#PBS -M email_address #PBS -m b	#BSUB -B	#@ notify_user = login_name #@ notification = start	sends email when job begins execution
#PBS -m e	#BSUB -N	#@ notification = complete	emails finished job report
#PBS -e errfile	#BSUB -e errfile	#@ error = errfile	redirects stderr to specified file
#PBS -o out_file	#BSUB -o out_file	#@ output = out_file	redirects stdout
	#BSUB -a application		esub parameter
#PBS -A project_name	#BSUB -P project_name	#@ account_no = project_name	assigns job to specified project
#PBS -l walltime=runtime	#BSUB -W runtime	#@ wall_clock_limit = runtime	sets the run limit of the job
#PBS -q queue_name	#BSUB -q queue_name	#@ class = queue_name	submit the job to the specified queue
#PBS -l select=[chunk specification]	#BSUB -n num_procs #BSUB -R "span[ptile=num_procs_per_node]"	#@ node = num_nodes #@ tasks_per_node = num_procs	specifies number of processors to use Specifies resource requirements an MPI job.

DAVINCI Queues Overview

Queue Name	Max Nodes/CPUs	Max Wall-Clock Time	Comments
transfer	1 node/ 1 CPUs	6 hrs.	Transfer jobs
standard	32 nodes256 CPUs	3 days	Non-challenge jobs
smp	1 node/32 CPUs	12 hrs.	Shared memory jobs
share	1 node/1 CPU	12 hrs.	Serial jobs.
challenge	128 nodes/1024 CPUs	7 days	Challenge & Priority Jobs
high	1 node/ 32 CPUs		
debug	32 nodes/256 CPUs	30 mins.	Debug Jobs
background	32 nodes/256 CPUs	4 hrs.	Negative Allocation jobs

```
#PBS -A NAVOSLMA                 # Charging Project ID.
#PBS -l walltime=04:00:00        # Wall clock time of 4 hours.
#PBS -q bigmem                   # Queue name.
#PBS -l select=1:ncpus=8         # Request one
                                 #8-processor "chunk"
#PBS -l place=excl               # Allocate node exclusively
#
# Run the OpenMP job with the IBM "poe" parallel job
starter.
```

Conclusion

Using PBS on the IBM P6 and CRAY XT systems should increase the efficiency of the systems and, therefore, the productivity of the NAVO MSRC users.

The NAVO MSRC User Support team is available to assist you with porting your LSF and/or LoadLeveler script to PBS Pro. Users are invited to direct requests for assistance to the Consolidated Customer Assistance Center (CCAC) at 1-877-222-2039 or by email at help@ccac.hpc.mil.

Environment Variable Comparison

PBS	LSF	LoadLeveler	Variable Description
PBS_JOBID	LSB_JOBID	LOADL_JOB_NAME	Unique job number.
PBS_ARRAY_INDEX	LSB_JOBINDEX	LOADL_STEP_ID	Job index for array jobs.
PBS_JOBNAME	LSB_JOBNAME	LOADL_STEP_COMMAND	Name of the job.
PBS_TASKNUM	LS_JOBPID	LOADL_PID	Process ID of the job.
PBS_ARRAY_ID			Identifier for job arrays. Consists of sequence number.
PBS_JOBDIR			Pathname of job-specific staging and execution directory.
PBS_JOBCOOKIE			Unique identifier for inter-MOM job-based communication.
PBS_QUEUE			The name of the queue from which the job is executed.
PBS_NODEFILE			The filename containing a list of vnodes assigned to the job.
PBS_NODENUM			Logical vnode number of this vnode allocated to the job.
PBS_ENVIRONMENT			Indicated job type: PBS_BATCH or PBS_ INTERACTIVE
PBS_MOMPORT			Port number on which this job's MOMs will communicate.
PBS_O_WORKDIR			The absolute path of the directory from which the job was submitted.
PBS_O_HOME			Value of HOME from submission environment.
PBS_O_LOGNAME			Value of LOGNAME from submission environment.
PBS_O_LANG			Value of LANG from submission environment.
PBS_O_PATH			Value of PATH from submission environment.
PBS_O_MAIL			Value of MAIL from submission environment.
PBS_O_QUEUE			The original queue name to which the job was submitted.
PBS_O_SHELL			Value of SHELL from submission environment.
PBS_O_HOST			The host name where qsub was executed.
PBS_O_SYSTEM			The operating system where qsub was executed.
PBS_O_TZ			Value of TZ from submission environment.
NCPUS			Number of threads, defaulting to number of CPUS, on the vnode.
OMP_NUM_THREADS			Same as NCPUS.
TMPDIR			The job-specific temporary directory for this job.

Coming Events

SNPD 09
Daegu, Korea
May 27 – 29, 2009

10th IEEE/ACIS International Conference on Software Engineering, Artificial Intelligence, Networking, and Parallel/Distributed Computing

IST 09
Shenzhen, China
May 9-10, 2009

IEEE International Workshop on Imaging Systems and Techniques

UGC 09
San Diego
June 15 - 18

http://www.hpcmo.hpc.mil/Htdocs/UGC/index.html

MSC 09
Saint Petersburg, RUSSIA
July 8-10, 2009

IEEE Multi-conference on Systems and Control

VIS 09
Atlantic City
October 11-16, 2009

Forum for visualization advances in science and engineering

ICCD 09
TBD

International Conference on Computer Design


NAVO Major Shared Resource Center
1002 Balch Boulevard, Stennis Space Center
Mississippi 39522