Project Status Report
High End Computing Capability
Strategic Capabilities Assets Program

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New Tool Provides Timely Analysis of Job Failures

- The HECC Application Performance & Productivity (APP) team has created a tool called “lumber” that facilitates rapid analysis of individual job failures by Control Room staff, and can help the overall system by allowing wholesale analysis of job failures.

- The tool gathers information from potentially thousands of separate log files pertaining to a given user job; it can gather this information for any job—typically within 30 seconds—automating a process that in the past was extremely laborious to the point of being unfeasible.

- Positive feedback from tool users includes:
  - “An easy-to-use tool that combines several time consuming steps.”
  - “Very helpful to diagnose job failures.”
  - “Enables timely response to user queries in a fast-paced environment.”
  - “Now an indispensable tool for finding job history.”

- Planned enhancements to the tool include the ability to diagnose and interpret the resulting job history to recognize known types of problems automatically, freeing up staff time that can be channeled into improving the overall system.

Mission Impact: The capability to perform timely and detailed log file analysis for jobs improves the delivery of HECC services to users, thus helping them meet their mission milestones on schedule and within budget.

Figure: The lumber tools traverses thousands of log files generated by executing jobs and stored at various places in the systems, to extract the information pertaining to a job. Note that some of these logged messages are not returned directly to the user in the course of normal execution.

POC: Dave Barker, david.p.barker@nasa.gov (650) 604-4292, NASA Advanced Supercomputing Division, Computer Sciences Corp.
The HECC Supercomputing Systems team has developed a utility to help users automate the reliable transfer of their data within the enclave and to external locations.

The utility, known as SHIFT (Self-Healing Independent File Transfer), selects the highest performance method to transfer the data, automatically validates data integrity, re-transmits data as needed, and provides status information to the user.

This automated process will reduce the effort spent on managing data transfers and allow HECC users to focus on their research, rather than on data transfer processes.

Implementation of the SHIFT utility will address user feedback on data transfers—one of the top areas of concern from the recent user survey (see HECC Project Report, 8 November 2011).

Mission Impact: Tools for automating reliable file transfers enable more efficient usage of scientific and engineering users’ time, and result in higher productivity.

POCs: Bob Ciotti, bob.ciotti@nasa.gov, (650) 604-4408, NASA Advanced Supercomputing Division; Davin Chan, davin.s.chan@nasa.gov, (650) 604-4613, NASA Advanced Supercomputing Division, Computer Sciences Corp. Paul Kolano, paul.kolano@nasa.gov, (650) 604-4271, NASA Advanced Supercomputing Division, Computer Sciences Corp.
HECC Deploys New Pleiades Filesystem Dedicated to Scientific Visualization

- HECC system engineers deployed a new Pleiades filesystem (designated p5) dedicated to visualization work; the new filesystem provides 1.7 petabytes (PB) of data storage space—quadrupling the storage capacity available for visualization.
- The new filesystem is identical to recently upgraded Pleiades hardware (see HECC Project Status Report, 10 January 1012), and provides the same 10-fold improvement in bandwidth and Input/Output Operations per Second (IOPS) performance.
- Systems experts deployed the filesystem with Lustre 2.1, the current major Lustre release; the remaining Pleiades filesystems will be migrated to the new release this year.
- With the new filesystem, the usable disk drive capacity on Pleiades has expanded to 6.8 PB (9.6 PB unformatted) of temporary storage space.

Mission Impact: Additional data storage capacity will allow NASA mission users to analyze more data-intensive models and simulations.

POCs: Bob Ciotti, bob.ciotti@nasa.gov, (650) 604-4408, NASA Advanced Supercomputing Division;
Davin Chan, davin.s.chan@nasa.gov, (650) 604-4613, NASA Advanced Supercomputing Division, Computer Sciences Corp.

Figure: The new Lustre filesystem on Pleiades provides a 10-fold increase in IOPS performance. Combined with increased hard drive storage density, the system delivers enhanced capabilities for scientific visualization.
Changes in Password Policy Ensure Compliance with Latest Requirements

• System administrators changed the password policy on HECC systems to comply with Security Control IA-5 (Authentication Management), specified in “National Institute of Standards and Technology Special Publication 800-53, Rev. 3,” required by NASA regulations.

• In compliance with Agency-defined values, the policy change requires that passwords:
  – Contain at least 3 of the 4 types of characters drawn from uppercase letters, lowercase letters, numbers, and special characters;
  – Contain at least 12 characters;
  – Have a minimum lifetime of 1 day and a maximum lifetime of 60 days;
  – Cannot be reused for 24 generations.

• When HECC users’ current passwords exceed the new 60-day limit, they will be required to change their passwords to meet the new requirements.

• The policy change-over, implemented on January 10, occurred seamlessly, with no issues.

Mission Impact: Compliance with Agency-wide security regulations protects NASA data and systems from unauthorized access.

Before: 8 characters

After: 12 characters

Figure: Longer passwords can still be easy to remember if they are based on a passphrase, with numbers substituted for vowels. While not required, an easy to remember, secure approach is to substitute numbers for vowels in a pass phrase such as “goodpassword” or “betterpassword” (truncated to the correct length, in the example above.)

POC: Thomas Hinke, thomas.h.hinke@nasa.gov, (650) 604-3662, NASA Advanced Supercomputing Division
HECC Network Utilization Tool Now Available Online

- HECC networking and web experts recently developed and launched a tool that shows real-time utilization on the front-end systems.
- All HECC users can now view network utilization levels of various front-end and storage systems via the HECC public website.
- Since many of the front ends hit 100% network utilization during peak hours, users’ transfer rates can be acutely impacted; this tool helps users choose specific systems to use based on the current load.
- The Networks team worked with the Publications & Media team on a method to get data pushed out every minute to the HECC website in a concise and easy-to-understand display.
- The front-end utilization tool can be viewed at: http://www.nas.nasa.gov/hecc/support/pfe_utilization.html

**Mission Impact:** Providing users with real-time information showing which front-end systems are under high network load allows them choose a less-utilized system to achieve faster data transfer rates.

**POCs:** Nichole Boscia, Nichole.K.Boscia@nasa.gov, (650) 604-0891; John Hardman, john.p.hardman@nasa.gov, (650) 604-0417, NASA Advanced Supercomputing Division, Computer Sciences Corp.

**Figure:** Screenshot showing various network utilization levels across the HECC front-end and storage systems.
In high-speed aerodynamics, shock wave/turbulent boundary layer interactions (STBLIs) can create intense heating and pressure loads that endanger aerospace vehicles or limit their designs.

Researchers in the NASA Advanced Supercomputing (NAS) Division are running large-eddy simulations (LES) to establish high-fidelity baseline solutions, quantify uncertainty levels, and improve STBLI modeling.

Simulation results have shown that a commonly observed discrepancy between previous simulation results and experimental measurements may be due to a 3D effect in the latter, rather than a difference in Reynolds number, as previously thought.

19 large-eddy simulations of an oblique shock impinging on a supersonic turbulent boundary layer were computed, using a range of parameters; calculations required approximately 3.3 million processor hours and would not have been possible without access to the Pleiades and Columbia supercomputers.

**Mission Impact:** HECC supercomputing resources, combined with a massive data storage capacity, enable advances in our understanding of turbulent flow physics and provide the engineering community with abilities to perform modeling and data analysis on a large scale not previously achievable.

**Figure:** An oblique shock impinges on an incoming turbulent boundary layer. Contours of the velocity gradient tensor are colored by streamwise momentum (blue indicates presence of reversed flow). Contours of negative dilatation (gray) are overlaid. Mach number = 2.28, Reynolds number = 2300. Brandon Morgan, Stanford University

**POC:** Nagi Mansour, nagi.n.mansour@nasa.gov, (650) 604-6420; NASA Advanced Supercomputing Division

HECC provided supercomputing resources and services in support of this work.
Simulations of the Solar Interior Help Understand the Sun’s Magnetic Cycle

- Using HECC resources, researchers at the University of Arizona are performing numerical simulations of the deep solar interior to better understand the dynamo mechanism by which all solar magnetic fields are created.
- Deciphering the dynamo mechanism is essential to predicting space weather and the impact of solar variability on the Earth.
- Studies of numerous, complex characteristics involved in self-consistent coupling of the Sun’s convective and radiative regions have revealed that hydrodynamic flows induced by convective overshoot (a phenomenon of convection carrying material beyond an unstable region of the atmosphere into a stratified, stable region) can limit the thickness of the solar tachocline, implying that an internal magnetic field does not contribute to the spread of the tachocline.
- Pleiades’ large computational capability and speed enables such intensive calculations and make this work possible.

**Mission Impact:** The availability of the Pleiades supercomputer contributes to NASA’s science goals by helping to interpret the Sun’s interactions with the Earth, and identifying causes of variance in the Sun.

**Figure:** Time snapshots of toroidal fields (a–d) and poloidal fields (e–g). In (a–d), white is a positive toroidal field, black is negative. Initially, in (a) the radial gradient of the differential rotation dominates the induction of the toroidal field. A toroidal field reversal in the tachocline and convection zone is seen between (b) and (c). A poloidal field is seen in (e–g) as it diffuses outward and decays over time. Color differences represent a steady increase in the toroidal field strength and steady decrease in the poloidal field strength. Tamara Rogers, University of Arizona

**POC:** Tamara Rogers, tami@lpl.arizona.edu, (520) 626-3338, University of Arizona

HECC provided supercomputing resources and services in support of this work
NASA Manager Completes High-Impact Term as Chair of HEC-IWG

- In January 2012, Dr. Bryan Biegel, Deputy Chief of the NASA Advanced Supercomputing (NAS) Division, completed a productive 1-year term as Chair of the High End Computing Interagency Working Group (HEC-IWG), under the Networking and IT R&D (NITRD) Subcommittee of the Office of Science and Technology Policy (OSTP).

- The HEC-IWG is charged with coordinating Federal investments and activities in HEC infrastructure and applications as well as HEC R&D; the HECC and NCCS projects are reported and coordinated as NASA investments within the scope of the HEC-IWG.

- During his term as HEC-IWG Chair, Dr. Biegel:
  - Began a new initiative to bring in expert speakers for each monthly meeting to present on topics important to the HEC-IWG
  - Organized a session on HEC software challenges and solutions at the Software Design and Productivity National Needs Summit
  - Organized a BoF session at SC11 on Agency research challenges and findings on scientific computing in the cloud
  - Created the first comprehensive archive of HEC-IWG activities and documents, covering his term as Chair
  - Led the HEC-IWG in selecting two important focus areas for coordination: supporting advanced manufacturing and facilitating a major update of HEC-related curricula and training
  - Dr. Biegel now is Vice-Chair of the HEC-IWG, to help the new Chair continue the positive impact of the HEC-IWG.

Mission Impact: Leading the HEC-IWG enables NASA to have a greater impact on the national HEC community, from supporting Congressional mandates to helping resolve shared challenges.

Figure: NASA played a significant role in a previous NITRD led activity: the 2003-4 development of the Federal Plan for High-End Computing by the High-End Computing Revitalization Task Force (HECRTF). This strategic plan influenced an ensuing dramatic expansion of HEC capacity at NASA and other agencies.

POC: Bryan Biegel, Bryan.Biegel@nasa.gov, (650) 604-0171, NASA Advanced Supercomputing Division
Status of Requests for NAS Computer Accounts by non-U.S. Citizens

- Requests approved: 8; New requests received: 8; Requests waiting: 8.
- Average wait time decreased because several outstanding requests were approved.
- Wait times are 0.7 – 3.1 months, with 1 over 3 months (applicant is from a designated country), and 2 over 1 month.
- The International Visitor Control Center has been contacted for updates on those who have been waiting more than one month.
HECC Facility Hosts Several Visitors and Tours in January 2012

- HECC hosted 2 scheduled tour groups in January; guests received an overview of the HECC Project, demonstrations of the hyperwall visualization system, and tours of the computer room floor. Guests this month included:
  - Jeri Buchholz, NASA Headquarters Assistant Administrator for Human Capital Management, who visited Ames and was briefed on the HECC Project and NASA Advanced Supercomputing facility by Bryan Biegel.
  - As part of the Ames New Workforce Orientation, 32 new staff members received a tour of the computer room, where they learned about the Agency-wide missions being supported by Pleiades, and viewed scientific results examined on the hyperwall-2 visualization system.

**Figure:** As part of the Ames Workforce Orientation, new staff members toured the NASA Advanced Supercomputing facility, which included a demonstration of the hyperwall-2.

**POC:** Gina Morello, gina.f.morello@nasa.gov, (650) 604-4462, NASA Advanced Supercomputing Division
Presentations and Papers

• 50th American Institute of Aeronautics and Astronautics (AIAA) Aerosciences Conference, Jan. 9–12, Nashville
  – “Inviscid Analysis of Extended Formation Flight,” J. Kless, M. Aftosmis, M. Nemec, A. Ning.*

  http://iopscience.iop.org/0004-637X/744/2/185/

* HECC provided supercomputing resources and services in support of this work
News and Events

  

- **SGI Books $90M in ICE X Super Orders**, *article, The Register*, Jan. 3, 2012 – Notes that NASA will be adding 1,700 Xeon E5 server nodes to Pleiades.
  
  http://www.theregister.co.uk/2012/01/11/sgi_ice_x_sales_barrenechea_board/
HECC Utilization Normalized to 30-Day Month

Standard Billing Units

February 2012

0
1,000,000
2,000,000
3,000,000
4,000,000
5,000,000
6,000,000

Alloc. to Orgs

SOMD
ESMD
NAS
NLCS
NESC
SMD
HEOMD
ARMD

High End Computing Capability Project
Allocation to orgs. decreased to 75%, Agency reserve shifted to ARMD

1. Allocation to orgs. decreased to 75%, Agency reserve shifted to ARMD
2. 14 Westmere racks added
3. 2 ARMD Westmere racks added
Tape Archive Status

Unique File Data | Unique Tape Data | Total Tape Data | Tape Capacity | Tape Library Capacity

January 2012
Tape Archive Status

1: LTO-4 -> LTO-5 migration
2: Library Expansion
3: LTO-4 media removed
4: LTO-5 media added
Pleiades: SBUs Reported, Normalized to 30-Day Month
Pleiades:
Devel Queue Utilization

Standard Billing Units


SOMD
ESMD
NAS
NLCS
NESC
SMD
HEOMD
ARMD
Devel Queue Alloc.
Pleiades:
Monthly SBUs by Run Time

*charge for reserved time

job run time (hours)

January 2012
Pleiades:
Monthly Utilization by Size and Mission

January 2012

*charge for reserved time

Job Size (cores)

Standard Billing Units

NAS
NLCS
NESC
SMD
HEOMD
ARMD
Pleiades: Monthly Utilization by Size and Length

January 2012

*charge for reserved time

**High End Computing Capability Project**
Pleiades: Average Expansion Factor

ARMD
HEOMD
SMD
NESC
ESMD
SOMD


5.85
27.13
Columbia:
SBUs Reported, Normalized to 30-Day Month
Columbia: Monthly SBUs by Run Time

- Standard Billing Units
- Job Run Time (hours)

January 2012

- 0 - 1 hours
- > 1 - 4 hours
- > 4 - 8 hours
- > 8 - 24 hours
- > 24 - 48 hours
- > 48 - 72 hours
- > 72 - 96 hours
- > 96 - 120 hours
- > 120 hours
Columbia: Monthly Utilization by Size and Mission

### Standard Billing Units

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January 2012
Columbia: Monthly Utilization by Size and Length

January 2012

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[Graph showing utilization by size and length for different job sizes and billing units for January 2012]
Columbia: Average Time to Clear All Jobs

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High End Computing Capability Project
Columbia: Average Expansion Factor


ARMD  HEOMD  SMD  NESC  ESMD  SOMD

5.15  6.94