Pleiades InfiniBand I/O Fabric Enhanced to Improve Performance and Reliability

- HECC engineers upgraded the I/O fabric on Pleiades to improve the performance and reliability of the I/O subsystem.
- The I/O fabric was changed from quad data rate (QDR) to fourteen data rate (FDR) InfiniBand (IB), which improved the reliability of the Lustre filesystems. Several of the recent storage outages were attributed to the instability of the QDR fabric.
- The new I/O fabric provides a 70% improvement in bandwidth per IB link, and the number of links increased by a factor of 2.2. The combined result is better connectivity to, and performance of, the Lustre filesystems.
- The filesystems migration occurred in two stages: two of the FDR-enabled filesystems were moved first to reap benefits from the improved bandwidth of the FDR I/O fabric, followed by migration of the remaining QDR-enabled filesystems.

**Mission Impact:** Ensuring a stable I/O fabric is essential for providing reliable high-performance computing resources to HECC users.

The Pleiades supercomputer’s fourteen data rate I/O fabric is comprised of 16 36-port Mellanox switches configured in a 4D hypercube.

POCs: Bob Ciotti, bob.ciotti@nasa.gov, (650) 604-4408, NASA Advanced Supercomputing (NAS) Division; Davin Chan, davin.chan@nasa.gov, (650) 604-3613, NAS Division, Computer Sciences Corp.
Data Migration Facility (DMF) Update Yields Significant Savings for HECC Program

- HECC engineers recently updated the Lou archive system to the latest version of DMF. In addition to improving Lou performance and reliability, this update changed how storage is licensed and saved $70K in licensing costs.

- HECC writes two copies of all user data to reduce the chances of data loss. One copy is written to the primary compute facility (Bldg. N258). The other is written to the secondary facility (N233A) located a kilometer away.

- Previously, all data managed by DMF was counted against the licensed capacity. The licensing agreement was changed to count only unique copies of the data, and as a result, doubled HECC’s licensed storage capacity. Without this change, HECC would need to procure additional licenses to keep up with a growth rate of 30% per year.

Mission Impact: With NASA’s rapidly growing data archiving requirements, HECC looks for opportunities to support storage requirements and minimize cost to the agency.

POCs: Bob Ciotti, bob.ciotti@nasa.gov, (650) 604-4408, NASA Advanced Supercomputing (NAS) Division; Davin Chan, davin.chan@nasa.gov, (650) 604-3613, NAS Division, Computer Sciences Corp.
APP Experts Facilitate Interactive Use of LDAN Nodes for Large-Memory Post-Processing

- In response to a user request, Application Performance and Productivity (APP) staff developed a procedure for running large, interactive post-processing jobs on the Lou Data Analysis (LDAN) nodes.
- Stephen Alter from the Aerothermodynamics Branch at NASA Langley Research Center needed to use Tecplot to produce Space Launch System (SLS) images for a review, but Pleiades front-end nodes did not have enough memory.
- The LDAN nodes have the required memory to accomplish the work, but several issues were encountered when trying to get Tecplot graphics to display on the user’s desktop. The APP team developed a procedure to work around them:
  - Set up a Virtual Network Computing (VNC) server on a Pleiades front-end node.
  - Use the ssh command from a terminal emulator launched in VNC to log into the LDAN allocated by the Portable Batch System scheduler.
- The APP team expects this procedure to be of help to other users, and is documenting them in the HECC Knowledge Base.

Mission Impact: HECC expertise in application performance and productivity makes it possible to address user issues quickly, enhancing productivity and contributing to mission success.

POC: Steve Heistand, steve.heistand@nasa.gov, (650) 604-4369, NASA Advanced Supercomputing Division, Computer Sciences Corp.
Normalized February Usage on Pleiades Sets New Monthly Record of 14.465 Million SBUs

- February’s normalized usage on the Pleiades supercomputer set a record of 14.465 million Standard Billing Units (SBUs*).
- Actual usage by NASA’s science and engineering organizations during the 28 days was over 13.5 million SBUs.
- Normalized usage exceeded the previous record (13.635 million SBUs in December 2014) by over 6%.
- This increase was enabled by the January 2015 addition of 1008 new Haswell nodes.
- Over 300 projects from across NASA used time on Pleiades during February.
- The top 10 projects used from 392,281 to 905,513 SBUs and together accounted for over 41% of total usage.
- The HECC Project continues to plan and evaluate ways to address the future requirements of NASA’s users.

*1 SBU equals 1 hour of a Pleiades Westmere 12-core node.

POC: Catherine Schulbach, catherine.h.schulbach@nasa.gov, (650) 604-3180, NASA Advanced Supercomputing Division
Simulations of Binary Star System ‘Eta Car’ Provide Insight into Stellar Colliding Winds *

- To gain understanding of binary colliding winds, researchers are running a 3D smoothed particle hydrodynamics (SPH) code on Pleiades to produce simulations of the supermassive stellar system Eta Carinae (Eta Car), famous for the largest non-terminal stellar explosion ever recorded.
- Simulations are used for direct comparison to observations by the Hubble Space Telescope (HST), Swift, Chandra, and Rossi X-ray Timing Explorer (RXTE). Key project results include:
  - First 3D-print model of Eta Car; reproduced observed RXTE X-ray light curve and HST optical spectra.
  - First determination of the 3D orientation of Eta Car’s binary orbit, and first direct evidence of the binary’s influence in shaping the Homunculus Nebula.
  - First HST images of stellar wind structures predicted by the simulations.
  - New understanding of how radiative forces in massive binaries affect the stars’ winds, colliding wind shocks, and variable X-ray emission.
- These simulations are made possible by NASA supercomputing resources. Continued work on Pleiades extends the Eta Car models to other massive colliding-wind binary systems.

* HECC provides supercomputing resources and services in support of this work

Mission Impact: Enabled by the Pleiades supercomputer, large 3D simulations have greatly increased our understanding Eta Carinae and massive colliding-wind binary systems in general.

Slices at different orbital phases ($\Phi$, columns) showing log density (g/cm$^3$, top row) and log temperature (K, bottom row) in the orbital plane from a 3D SPH simulation of Eta Car's binary colliding winds. The simulation domain radius is 155 AU (1 AU equals the distance between the Sun and the Earth). The stellar separation is largest at apastron and smallest at periastron. The stars and wind-wind collision region (WWCR) are marked in the rightmost panel.

POCs: Thomas Madura, thomas.i.madura@nasa.gov, (301) 286-7628, Theodore Gull, theodore.r.gull@nasa.gov, (301) 286-6184, NASA Goddard Space Flight Center
HECC Resources Enable Extensive CFD Analyses for SLS Wind Tunnel Booster Separation Model *

- NASA Advanced Supercomputing (NAS) Division modeling and simulation experts completed extensive computational fluid dynamics (CFD) simulations of booster separation for the Space Launch System (SLS) wind tunnel model.
  - Modeled the SLS booster separation wind tunnel model.
  - Performed over 8,000 Cart3D simulation cases, covering a wide range of booster separation positions and Mach numbers, with and without booster separation motor plumes.
  - Computed aerodynamic forces, moments, surface pressures, and line loads on the boosters and core stage, and compared results with wind tunnel data.
  - Performed high-fidelity, viscous OVERFLOW simulations of 12 key cases to investigate differences between wind tunnel and simulation data.
  - Determined that wind tunnel data anomalies are due to unknown interference or facility effects.
- These extensive analyses required around 90,000 processor-hours on the Pleiades supercomputer, and produced valuable aerodynamic data for the SLS booster separation database.

Mission Impact: Enabled by HECC resources, computational fluid dynamics analyses of SLS booster separation provide critical aerodynamic data needed to design safe, effective separation systems and assess potential risks of recontact with the core stage.

Snapshot from a Cart3D simulation of booster separation flow. The surface is colored by pressure, and the gray-scale flow contours show the booster-separation motor plumes.

POC: Stuart Rogers, stuart.e.rogers@nasa.gov, (650) 604-4481, NASA Advanced Supercomputing Division

* HECC provides supercomputing resources and services in support of this work
Simulations Enhance Space Launch System
Scale Model Acoustic Test Analyses *

• Researchers are running computational fluid dynamics (CFD) simulations on Pleiades to better understand and interpret Space Launch System (SLS) Scale Model Acoustic Test (SMAT) data and to gain additional insight into the predicted flow physics of the SLS launch environment.
  – Extensive testing and analysis are required to ensure that acoustic pressure waves generated during liftoff will not compromise the vehicle. The SMAT uses a 5% scale model of the SLS to help predict the acoustic launch environment and assess the effectiveness of the launch platform’s water sound suppression system.
  – The CFD simulations are performed in conjunction with the SMAT tests to enable full analysis of the 3D fluid dynamics around the scale model (test data is not recorded at all locations), help distinguish different sources of overpressure waves, and investigate effects of timing variations in solid rocket booster ignition.
• The simulation results provide key data needed to help engineers design the SLS and its water sound suppression system to assure safe liftoffs.
• SMAT data will also be used to validate the simulation methods for future analysis of the full-scale SLS launch environment.

Mission Impact: HECC resources enabled large CFD simulations to be completed in just weeks, allowing researchers adequate time to assess their results and provide feedback to test engineers during the SLS Scale Model Acoustic Test.

The Space Launch System Scale Model Acoustic Test is shown (right) next to a computational fluid dynamics (CFD) simulation of the model (left). The CFD image shows contours of the pressure gradient magnitudes, which accent the overpressure waves surrounding the vehicle during the early stages of a launch simulation.

POCs: Tanner Nielsen, tanner.b.nielsen-1@nasa.gov, (256) 544-6330, NASA Marshall Space Flight Center, Jacobs Technology

* HECC provided supercomputing resources and services in support of this work
HECC Facility Hosts Several Visitors and Tours in February 2015

- HECC hosted 15 tour groups in February; guests learned about the agency-wide missions being supported by HECC assets, and some of the groups also viewed the D-Wave Two quantum computer system. Visitors this month included:
  - His Excellency Xavier Bettel, Prime Minister of Luxembourg, and Mohammad Ghoniem, Luxembourg Institute of Science and Technology (LIST), as part of a continuing collaboration on big data and visualization methods used at the NAS facility.
  - 20 students from the Lassen Astrobiology Internship Program (Red Bluff High School, Lassen, CA) visited Ames Research Center (ARC) as part of their courses on science and mathematics.
  - A group of 20 NASA researchers attending the Rodent Research 2 Delta Operations Verification Test held at ARC visited as part of their center tour.
  - 30 participants of the Ames education enrichment programs who are currently interning at ARC visited the facility to learn more about computational fluid dynamics (CFD) and supercomputing.
  - A group of 16 students from the Society of Hispanic Professional Engineers at California Polytechnic State University, who are studying CFD courses, visited ARC to learn more about NASA research and possible internship opportunities for summer programs.

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

  http://scitation.aip.org/content/aip/journal/pop/22/2/10.1063/1.4908545
  http://arxiv.org/abs/1502.02052
  http://journals.ametsoc.org/doi/abs/10.1175/JAMC-D-14-0216.1
  http://iopscience.iop.org/0004-637X/800/2/87
  http://spie.org/Publications/Proceedings/Paper/10.1117/12.2083256

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

• **NASA Supercomputer Intensifies Exomoon Search**, *HPCwire*, February 11, 2015—A team at Harvard University has launched the Hunt for Exomoons with Kepler (HEK) project to find moons that might support life. Utilizing the Pleiades supercomputer to sort through Kepler data, the team developed a unique computational method based on light-curve modeling algorithms to identify exomoons orbiting Kepler planet candidates. (Original NASA feature reported in January 2015.)
  
HECC Utilization Normalized to 30-Day Month
HECC Utilization Normalized to 30-Day Month

![Graph showing HECC utilization normalized to 30-day month with details on equipment additions and retirements.]

- **SMD**
  - Standard Billing Units in Millions
  - Bars represent monthly utilization from March 2013 to February 2015.
  - Key events:
    1. Columbia 22 retired; Endeavour 1 added
    2. 32 Harpertown Racks retired
    3. 32 Harpertown Racks retired; 46 Ivy Bridge Racks added
    4. 6 Ivy Bridge Racks added; 20 Nehalem, 12 Westmere Racks Retired
    5. 8 Ivy Bridge Racks added mid-Feb; 8 Ivy Bridge Racks added late Feb.
    6. 4 Ivy Bridge Racks added mid-March
    7. 6 Westmere Racks added to Merope, Merope Harpertown retired
    8. 16 Westmere Racks retired; 10 Nehalem Racks and 2 Westmere Racks added to Merope; 3 Ivy Bridge Racks added; 15 Haswell Racks added
    9. 16 Westmere Racks retired
    10. 14 Haswell racks added

- **HEOMD, NESC**
  - Standard Billing Units in Millions
  - Bars represent monthly utilization from March 2013 to February 2015.

- **ARMD**
  - Standard Billing Units in Millions
  - Bars represent monthly utilization from March 2013 to February 2015.
  - Key events:
    1. ARMD Allocation
    2. SMD Allocation

National Aeronautics and Space Administration

Mar 10, 2015

High-End Computing Capability Project
Pleiades: SBUs Reported, Normalized to 30-Day Month
Pleiades: Devel Queue Utilization

![Chart showing Devel Queue utilization over time with different billing units and departments]
Pleiades: Monthly Utilization by Job Length

February 2015

<table>
<thead>
<tr>
<th>Job Run Time (hours)</th>
<th>Standard Billing Units</th>
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<td>&gt; 48 - 72 hours</td>
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<td>&gt; 72 - 96 hours</td>
<td>1,800,000</td>
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<tr>
<td>&gt; 96 - 120 hours</td>
<td>1,500,000</td>
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<tr>
<td>&gt; 120 hours</td>
<td>1,000,000</td>
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Pleiades: Monthly Utilization by Size and Mission

February 2015
Pleiades: Monthly Utilization by Size and Length

February 2015

Job Size (cores)

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<tr>
<th>Standard Billing Units</th>
<th>0 - 1 hours</th>
<th>1 - 4 hours</th>
<th>&gt; 4 - 8 hours</th>
<th>&gt; 8 - 24 hours</th>
<th>&gt; 24 - 48 hours</th>
<th>&gt; 72 - 96 hours</th>
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Pleiades:
Average Time to Clear All Jobs


Hours

ARMD  HEOMD/NESC  SMD
Pleiades:
Average Expansion Factor

ARMD 6.63
HEOMD 15.87
SMD 9.06
Endeavour: SBUs Reported, Normalized to 30-Day Month
Endeavour: Monthly Utilization by Job Length

February 2015
Endeavour: Monthly Utilization by Size and Mission

February 2015
**Endeavour: Monthly Utilization by Size and Length**

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<table>
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<td>&gt; 4 - 8 hours</td>
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<td>&gt; 1 - 4 hours</td>
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<tr>
<td>0</td>
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February 2015
Endeavour: Average Time to Clear All Jobs

- **ARMD**
- **HEOMD/NESC**
- **SMD**
Endeavour: Average Expansion Factor

ARMD
HEOMD
SMD
Merope: SBUs Reported, Normalized to 30-Day Month
Merope: Monthly Utilization by Job Length

![Graph](image)

February 2015
Merope:
Monthly Utilization by Size and Mission

February 2015
Merope:
Monthly Utilization by Size and Length

February 2015
Merope:
Average Expansion Factor

![Bar chart showing average expansion factors for ARMD, HEOMD, and SMD from March 2014 to February 2015.](image-url)