Project Status Report

High End Computing Capability
Strategic Capabilities Assets Program

February 10, 2017

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Applications Team Characterizes I/O Performance of New Electra Supercomputer

- HECC’s Application Performance and Productivity (APP) team conducted extensive testing of I/O performance on the new Electra supercomputer.
- Electra is housed in the Modular Supercomputing Facility (MSF) adjacent to Bldg. N258, and has no user filesystems co-located with it. Instead, it connects to filesystems in the main facility via a network that uses MetroX InfiniBand extenders and Lustre routers.
- The uniqueness of this setup necessitated extensive testing to ensure that application I/O performance would be similar to what users experience on Pleiades.
  - The APP team investigated the sensitivity of I/O performance to the number of Lustre routers used to connect to the filesystems.
  - They found that using 10 Lustre routers for Electra provided equivalent performance to jobs running on Pleiades.
- Future expansion of the MSF can be accommodated over the existing infrastructure, potentially adding additional MetroX links and Lustre routers if needed.

Mission Impact: Extensive testing to evaluate I/O performance reduces risks associated with the new deployment and enables HECC to provide better advice to users seeking to optimize code performance.

Electra supercomputer users get access to their files in the main facility via Mellanox MetroX MTX6000 InfiniBand extenders, which connect the Electra fabric in the Modular Supercomputing Facility to Lustre routers on the InfiniBand fabric in the NAS facility over 16 fiber optic links, each about 1,000 feet long.

POCs: Henry Jin, haoqiang.jin@nasa.gov, NASA Advanced Supercomputing (NAS) Division; Robert Hood, robert.hood@nasa.gov, NAS Division, CSRA LCC
Highly Parallel Input/Output Routines in MITgcm Demonstrate MSF Capabilities

- HECC visualization experts developed highly parallel input/output routines to enable extremely high-resolution ocean modeling runs on 30,000 cores of Electra, accessing filesystems on Pleiades’ network, using the high-end MIT General Circulation Model (MITgcm) employed by the Estimating the Circulation and Climate of the Ocean (ECCO) project team.

- Newly developed input routines, using industry-standard MPI-IO, cut model startup times from hours to minutes.
  - 1.5 terabytes (TB) of input data was read and distributed across 30,000 compute ranks in less than 5 minutes.

- Custom output routines, developed from the Visualization team’s concurrent visualization framework, enabled filesystem writes at hardware speeds.
  - Combined diagnostic and checkpoint output of greater than 2 TB was written in less than 2 minutes, with peak rates of ~45 gigabytes per second (GB/s).

- The team used the high-bandwidth MITgcm application to stress-test the network connections between Electra and the Pleiades filesystems.

- MITgcm application was able to take full advantage of the newly deployed Electra/Pleiades capabilities to enable scientifically useful computations at unprecedented detail and resolution.

Mission Impact: HECC’s extreme-scale deployment of a highly optimized code confirmed the excellent performance and utility of the MSF installation, and enabled new science with a community-standard model run at unprecedented resolution.

Tiny piece of a computational domain shows swirling temperature variations at 250 meters/pixel just outside San Francisco Bay.  
Chris Henze, NASA/Ames

POCs: Chris Henze, chris.henze@nasa.gov, (650) 604-395, NASA Advanced Supercomputing (NAS) Division; Bron Nelson, bron.c.nelson@nasa.gov, (650) 604-4329, NAS Division, CSRA LLC
HECC Implements Cost-Effective Expansion of Merope Supercomputer

- HECC engineers completed an expansion of the Merope supercomputer with 640 additional Westmere nodes. This represents a 55% increase in computing capacity on Merope.
- The expansion comprises repurposed Westmere nodes retired from Pleiades to provide the power and cooling necessary for the Broadwell augmentation to Pleiades.
- The nodes were integrated into Merope during a system maintenance downtime. Due to floor-load constraints, the nodes are housed in 20 half-populated racks.
- In addition to providing computational resources to HECC users, the Merope cluster serves as a platform for large-scale system tests that could adversely impact users on Pleiades.

Mission Impact: Repurposing retired hardware enables HECC to cost-effectively deliver additional computational cycles to NASA users.

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, CSRA LLC
HECC Account Request System Enhanced to Improve RSA Token Renewal Requests

• The HECC Tools team enhanced the Account Request System to include the capability for users to renew their expiring RSA tokens online, eliminating the need for staff to manually contact users for upcoming renewals. The HECC Accounts team now send users with expiring tokens the Account Request System link to renew their tokens.

• Development of the token renewal feature included:
  – Parsing the RSA token information from the Radius database.
  – Developing options to allow users to select soft tokens (iOS or Android) or token fobs.
  – Obtaining correctly formatted mailing addresses for hard tokens and providing detailed emails and instructions for setting up the multiple steps necessary for soft tokens.

• Future plans include developing a screencast for the soft token setup, and automating user notifications based on the token expiration date.

Mission Impact: Online renewal of NASA’s required two-factor authentication RSA tokens provides a streamlined workflow for ensuring that token renewals are efficiently handled for HECC users.

POC: Ryan Spaulding, ryan.c.spaulding@nasa.gov, (408) 772-6567, NASA Supercomputing Division, ADNET Systems
HECC Support Staff Continue Providing Excellent Help to Users

- In 2016, HECC staff provided support to more than a thousand users from all of NASA’s mission directorates.
- Support staff across the HECC project processed, tracked, and resolved over 21,000 tickets for the 12 months from January 1, 2016 through December 31, 2016.
- Tickets covered a wide range of support activities—from automated notifications of system issues to resolving a variety of issues for users calling for help:
  - Answered inquiries about accounts, failed jobs, and status of systems.
  - Extended run-times of already-queued or running jobs.
  - Modified allocations and account expiration dates.
  - Explained file transfer tools and processes.
  - Debugged job failures and identifying execution bottlenecks.

Mission Impact: The 24x7 support services provided by HECC experts resolve system problems and users’ technical issues, and enable users to focus on their critical mission projects.

POC: Leigh Ann Tanner, leighann.tanner@nasa.gov, (650) 604-4468, NASA Advanced Supercomputing Division, CSRA LLC

Number of Tickets Closed in 2016

HECC staff typically resolved just under 1,800 Remedy tickets per month in 2016—just over 21,000 tickets total.
January 2017 HECC Supercomputer Usage Sets New High of 22.76 Million SBUs

- In January, combined usage on HECC supercomputers set a new record.
- 22,757,811 Standard Billing Units (SBUs*) were used on Pleiades, Electra, Merope, and Endeavour by NASA’s science and engineering organizations.
- Usage exceeded by about half a million SBUs the previous record of 22.3 million set in December 2016.
- This increase was enabled by the addition of Electra and the expansion of Merope.
- Over 310 projects from all across NASA used time on one or more HECC systems.
- The top 10 projects used from 459,306 to 3,188,080 SBUs each and together accounted for over 43% of total usage.
- The HECC Project continues to plan and evaluate ways to address the future requirements of NASA’s users.

**Mission Impact:** Increasing capacity of HECC systems provides Mission Directorates with more resources for the accomplishment of their goals and objectives.

*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
Improving Fidelity of Launch Vehicle Liftoff Acoustic Simulations *

- Researchers at Marshall Space Flight Center (MSFC) used a hybrid CFD and computational aero-acoustics (CFD/CAA) modeling framework to simulate highly complex plume formation and interaction with launch pad geometry to accurately model the reflection and refraction of acoustic waves on launch pad components.
- The MSFC team’s CFD/CAA code was developed to improve such liftoff acoustic environment predictions and optimized for running on Pleiades.
  - The new CFD/CAA approach proved highly capable of accurately propagating and conserving the acoustic wave field over the complex launch vehicle and launch pad geometry.
  - Numerical simulations can be applied in evaluating various sound suppression measures, reducing the need for expensive testing.
- HECC supercomputing resources are instrumental in completing this type of analysis. The model requires ~300 million mesh cells to simultaneously resolve the launch vehicle and launch pad details and adequately capture the acoustic sources at the rocket plumes.

Mission Impact: Enabled by the Pleiades supercomputer, the improved capability to perform high-fidelity computational acoustic field simulations will increase confidence in the characterization of launch acoustic loads environments through computational modeling.

POCs: Peter Liever, peter.a.liever@nasa.gov, (256) 544.3288, Jeff West, jeffrey.s.west@nasa.gov, (256) 544.6309, NASA Marshall Space Flight Center

* HECC provided supercomputing resources and services in support of this work
Running Simulations on Pleiades to Improve Engineering Models for Aerospace Design *

- Predicting the behavior of turbulent flow passing over an aircraft or spacecraft is one of the most important tasks involved in designing such vehicles. It is also one of the most difficult.
- To improve engineering turbulence models, researchers at NASA Langley are running turbulent flow simulations on Pleiades to obtain high-fidelity benchmark data needed for more accurate models.
  - A family of cases was obtained by computing the equations governing the flow over a smooth flat surface, under conditions representative of air passing over a flight vehicle.
  - Conditions were adjusted to produce separation of the turbulent boundary layer (air adjacent to the surface), enabling the analysis of one of the most important and difficult-to-model features of an aerodynamic flow.
- Results are being used to quantify the shortcomings of current turbulence models and identify improvements required for next-generation models.
- These improvements could lead to superior vehicle design, in terms of flight characteristics and fuel efficiency, as well as lower the risk and cost of future aircraft and space vehicles.

Mission Impact: Run on HECC resources, these simulations support the Transformational Tools & Technologies Project of NASA's Transformative Aeronautics Concepts Program, helping to develop computational tools to design aerospace vehicles.

POCs: Gary Coleman, gary.n.coleman@nasa.gov, (757) 864-5486, Christopher Rumsey, c.l.rumsey@nasa.gov, (757) 864-2165, NASA Langley Research Center

* HECC provided supercomputing resources and services in support of this work.
HECC Facility Hosts Several Visitors and Tours in January 2017

• HECC hosted 11 tour groups in January; guests learned about the agency-wide missions being supported by HECC assets, and some groups also viewed the D-Wave 2X quantum computer system. Visitors this month included:
  – Meg Whitman, President and Chief Executive Officer of Hewlett Packard Enterprise, and several members of her team, were briefed by Ames executive management and visited the NAS facility.
  – Mike Mastaler, Director of the NASA Space Environments Testing Management Office (STEMO) received Ames executive management reviews and a Center tour that included the HECC Modular Supercomputing Facility.
  – David Horner, Director, Department of Defense (DoD), High Performance Computing Modernization Program (HPCMP), and Sandy Landsberg, Deputy Director, DoD HPCMP, had discussions with HECC/NAS management about HPC at NASA to explore areas of mutual interest.
  – David Hazlehurst, Australia’s Deputy Secretary for Industry, Innovation & Science and a group from that office received a executive management review that included the NAS Facility.
  – Mark Glorioso, Director, NASA Shared Services Center.
  – Andy Schain, Data Integration Integrated Task Team lead for the Exploration Systems Division.
  – 20 new civil servants hired at Ames.

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

  https://arxiv.org/abs/1701.00814

  http://www.the-cryosphere-discuss.net/tc-2016-288/tc-2016-288.pdf


  - “Computational Fluid Dynamics Analyses for the High-Lift Common Research Model Using the USM3D and FUN3D Flow Solvers,” M. Rivers, C. Hunter, V. Vasta. *

* HECC provided supercomputing resources and services in support of this work
Papers (cont.)

- **AIAA SciTech Forum (cont.)**
  - “Large Eddy Simulations of High Pressure Jets: Effect of Subgrid Scale Modeling,” J. Bellan, A. Gnanaskandan. *
  - “Advanced Modeling of Non-Equilibrium Flows Using a Maximum Entropy Quadratic Formulation,” M. Priyadarshini, Y. Liu, M. Panesi. *
  - “Numerical Investigation of Vibrational Relaxation Coupling with Turbulent Mixing,” R. Fievet, S. Voelkel, V. Raman, P. Varghese. *
  - “Optical Flow for Flight and Wind Tunnel Background Oriented Schlieren Imaging,” N. Smith, J. Heineck, E. Schairer. *

* HECC provided supercomputing resources and services in support of this work
• AIAA SciTech Forum (cont.)
  – “Retroreflective Background-Oriented Schlieren Imaging Results from the NASA Plume/Shock Interaction Test,” N. Smith, D. Durston, J. Heineck. *

• “Optimal Numerical Solvers for Transient Simulations of Ice Flow Using the Ice Sheet System Model (ISSM versions 4.2.5 and 4.11),” F. Habbal, et al., Geoscientific Model Development, vol. 10, January 10, 2017. *
  http://www.geosci-model-dev.net/10/155/2017/


  https://arxiv.org/abs/1701.03792

* HECC provided supercomputing resources and services in support of this work
Papers (cont.)


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

  - “Nozzle Plume/Shock Interaction Sonic Boom Test Results from the NASA Ames 9- by 7-Foot Supersonic Wind Tunnel,” D. Durston, S. Cliff, M. Denison, D. Dalle, et al. *

* HECC provided supercomputing resources and services in support of this work
Presentations (cont.)

- **AIAA SciTech Forum (cont.)**

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

- **Exploring Drone Aerodynamics with Computers**, *NASA Ames Feature*, January 11, 2017—Simulations of popular, commercial quadrotor drones performed by researchers on the Pleiades supercomputer show airflow interactions that offer new insights into the design of more efficient autonomous, heavy-lift, multirotor vehicles.
  
  https://www.nasa.gov/image-feature/ames/exploring-drone-aerodynamics-with-computers

    http://insidehpc.com/2017/01/drone-aerodynamics/

    http://www.dailymail.co.uk/sciencetech/article-4125220/Nasa-releases-animation-showing-airflow-drones.html

    https://www.wired.com/2017/01/stunning-animation-reveals-air-swirling-around-drone/

  – **Have a quadcopter drone? Check out its aerodynamics**, *Cosmos Magazine*, February 1, 2017.
    https://cosmosmagazine.com/physics/drone-aerodynamics
HECC Utilization Normalized to 30-Day Month

Standard Billing Units

NAS
NLCS
NESC
SMD
HEOMD
ARMD
Alloc. to Orgs

Alloc. to Orgs
HECC Utilization Normalized to 30-Day Month

1. 7 Nehalem ½ racks retired from Merope
2. 7 Westmere ½ racks added to Merope
3. 16 Westmere racks retired from Pleiades
4. 10 Broadwell racks added to Pleiades
5. 4 Broadwell racks added to Pleiades
6. 14 (All) Westmere racks retired from Pleiades
7. 14 Broadwell Racks added to Pleiades
8. 16 Electra Broadwell Racks in Production, 12 Westmere 1/2 racks added to Merope
Tape Archive Status

![Graph showing tape archive status with various metrics: Tape Library Capacity, Tape Capacity, Total Tape Data, Unique Tape Data. The graph tracks data from February 2015 to January 2017.](image-url)
Pleiades: SBUs Reported, Normalized to 30-Day Month
Pleiades: Devel Queue Utilization

![Graph showing Devel Queue Utilization from February 2016 to January 2017 with various agencies' billing units.

- Standard Billing Units
- NAS
- NLCS
- NESC
- SMD
- HEOMD
- ARMD
- Devel Queue Alloc.
Pleiades: Monthly Utilization by Job Length

![Bar chart showing monthly utilization by job length for Pleiades in January 2016. The x-axis represents job run time in hours, categorized into intervals: 0 - 1 hours, > 1 - 4 hours, > 4 - 8 hours, > 8 - 24 hours, > 24 - 48 hours, > 48 - 72 hours, > 72 - 96 hours, > 96 - 120 hours, and > 120 hours. The y-axis represents standard billing units, ranging from 0 to 6,000,000. The chart shows a significant increase in utilization for jobs with run times greater than 120 hours.]
Pleiades: Monthly Utilization by Size and Mission

January 2016
Pleiades:
Monthly Utilization by Size and Length

![Bar chart showing the monthly utilization of Pleiades by job size (cores) and length of time. The chart includes categories for different billing hours, ranging from 0-1 hours to >120 hours.](image-url)

January 2016
Pleiades:
Average Time to Clear All Jobs

Hours

ARMD
HEOMD/NESC
SMD
Pleiades:
Average Expansion Factor

February 10, 2017
Electra:
SBUs Reported, Normalized to 30-Day Month
Electra:
Devel Queue Utilization

- Standard Billing Units

- NAS
- NLCS
- NESC
- SMD
- HEOMD
- ARMD

Devel Queue Allocation

Electra: Monthly Utilization by Job Length

January 2016

Job Run Time (hours)

- 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

Standard Billing Units

- 0
- 250,000
- 500,000
- 750,000
- 1,000,000
- 1,250,000
- 1,500,000
Electra: Monthly Utilization by Size and Mission
Electra: Monthly Utilization by Size and Length

January 2016
Electra:
Average Time to Clear All Jobs

![Graph showing the average time to clear all jobs for different months. The x-axis represents the months from February 2016 to January 2017, and the y-axis represents the hours. The graph has three categories: ARMD, HEOMD/NESC, and SMD. The bar for January 2017 is significantly higher than the others, indicating a significant increase in the time to clear all jobs.]
Electra: Average Expansion Factor
Merope:
SBUs Reported, Normalized to 30-Day Month

Standard Billing Units

Feb-16  Mar-16  Apr-16  May-16  Jun-16  Jul-16  Aug-16  Sep-16  Oct-16  Nov-16  Dec-16  Jan-17

Alloc. to Orgs

NAS  NLCS  NESC  SMD  HEOMD  ARMD

0  250,000  500,000  750,000  1,000,000  1,250,000  1,500,000

February 10, 2017

High-End Computing Capability Project
Merope: Monthly Utilization by Job Length

<table>
<thead>
<tr>
<th>Job Run Time (hours)</th>
<th>Standard Billing Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>0 - 1 hours</td>
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<tr>
<td>&gt; 1 - 4 hours</td>
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<td>&gt; 4 - 8 hours</td>
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<td>&gt; 8 - 24 hours</td>
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</tbody>
</table>

January 2016
Merope:
Monthly Utilization by Size and Mission

January 2016
Merope:
Monthly Utilization by Size and Length

January 2016
Merope: Average Time to Clear All Jobs

![Bar chart showing average time to clear all jobs from February 2016 to January 2017. The x-axis represents months, and the y-axis represents hours. The chart shows data for ARMD, HEOMD/NESC, and SMD. The average time to clear all jobs varies across the months, with some months having significantly higher times. Notably, January 2017 has an average time of 160 hours.]
Merope: Average Expansion Factor

![Bar chart showing average expansion factor from Feb-16 to Jan-17 for ARMD, HEOMD, and SMD departments. The vertical axis represents the factor ranging from 1.00 to 7.00. Each month from Feb-16 to Jan-17 is plotted with corresponding bars for each department. The chart indicates fluctuations in expansion factors across different months.]
Endeavour: SBUs Reported, Normalized to 30-Day Month


Endeavour:
Monthly Utilization by Job Length

[Bar chart showing job run time distribution for January 2016]

- 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

Standard Billing Units

Job Run Time (hours)
Endeavour:
Monthly Utilization by Size and Mission

January 2016
Endeavour: Monthly Utilization by Size and Length

January 2016
Endeavour: Average Time to Clear All Jobs

![Bar chart showing average time to clear all jobs for different months from Feb-16 to Jan-17. The chart includes three categories: ARMD, HEOMD/NESC, and SMD.]
Endeavour:
Average Expansion Factor

![Graph showing average expansion factor from February 2016 to January 2017. The graph compares ARMD, HEOMD, and SMD over the months. The highest values are observed in November 2016.](image-url)