Project Status Report

High End Computing Capability
Strategic Capabilities Assets Program

September 10, 2014

Dr. Rupak Biswas – Project Manager
NASA Ames Research Center, Moffett Field, CA
Rupak.Biswas@nasa.gov
(650) 604-4411

HECC Resources Restored to Full Capacity After Cooling System Repairs

- After operating at half capacity since mid-July, when a cooling system failure reduced the cooling capability at the NASA Advanced Supercomputing (NAS) facility, HECC computing resources were returned to full operations on August 18.
  - During the period of reduced cooling capability, HECC system engineers operated the Pleiades supercomputer with half of its Ivy Bridge, Sandy Bridge, and Westmere nodes in order to provide users with the mix of processors required to run their jobs.
  - The User Services team also worked with Mission Directorate managers to ensure that critical work was prioritized.
- After the cooling system repairs were completed (see slide 8), HECC systems engineers were able to bring resources back online quickly, with no additional downtime.

Mission Impact: Restoring the Pleiades supercomputer to full capacity ensures that researchers across all NASA mission directorates have the high-end computing resources they need to accomplish their science and engineering goals.

The Pleiades supercomputer operated at half capacity while two damaged cooling pumps at the NAS facility were extracted and repaired offsite. HECC system engineers quickly made Pleiades fully operational for agency users after the pumps were reinstalled.

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.

Merope Upgraded with Intel Westmere Nodes Repurposed from Pleiades

- HECC systems engineers recently upgraded the Merope supercomputer, replacing the system's Harpertown nodes with Westmere nodes that were retired when Pleiades was upgraded with Ivy Bridge nodes.
- With the upgrade, Merope is now configured with 16 half-populated Westmere racks that contain 512 nodes, with a total of 6,144 cores and 12 terabytes of memory.
- When Merope is not being used for InfiniBand network and system testing, it provides additional computational resources to HECC users. The upgrade nearly doubles the number of Standard Billing Units (SBUs)* that Merope can deliver.
- Merope is in the process of being augmented further with 6 half-populated Westmere racks and 14 Nehalem racks that were also retired from Pleiades.

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

Mission Impact: Repurposing hardware enables HECC engineers to test system changes and enhancements to the Pleiades supercomputer without impacting users' job, and delivers additional computational cycles to scientists and engineers.

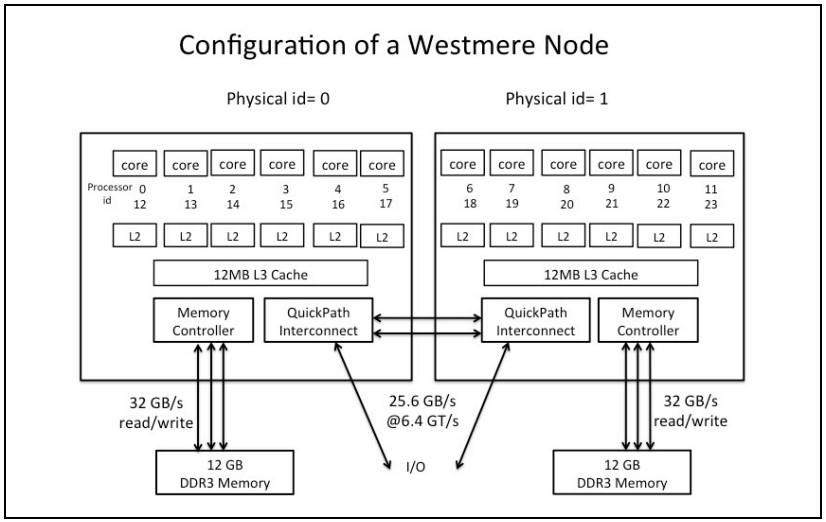
The Merope supercomputer, located in the auxiliary NAS facility, is used for InfiniBand network and system testing, and provides additional computing resources for users.

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, Computer Sciences Corp.

HECC Team Identifies Performance Issues, Optimizes Job Efficiency for Pleiades Users

- Experts in the HECC Application Performance and Productivity (APP) group provided code optimization services to improve job efficiency for seven Pleiades users, achieving results ranging from a 20% reduction in job execution times to a 10-fold improvement in parallel efficiency.
- The APP team identified jobs running on Pleiades that did not use all the cores on their allocated nodes, then contacted the users and provided them with code changes. The team found that:
  - In some cases, users left cores idle because the large memory requirements of their jobs allowed only a few processes to run on each node. The code changes provided by the APP team reduced cache and memory bandwidth contention by appropriately pinning processes on each node.
  - In one case, a user intended to run 80 sequential jobs across 10 nodes, but incorrect scripting left 9 nodes idle for the duration of the 120-hour job. The team helped this user achieve a 10-fold improvement in efficiency.
- The APP team also provided training to help these users learn to modify their own scripts in the future.

Mission Impact: HECC's customized code optimization services enable researchers to better utilize NASA's supercomputing resources and improve turnaround times for their modeling and simulation projects supporting the agency's mission goals.



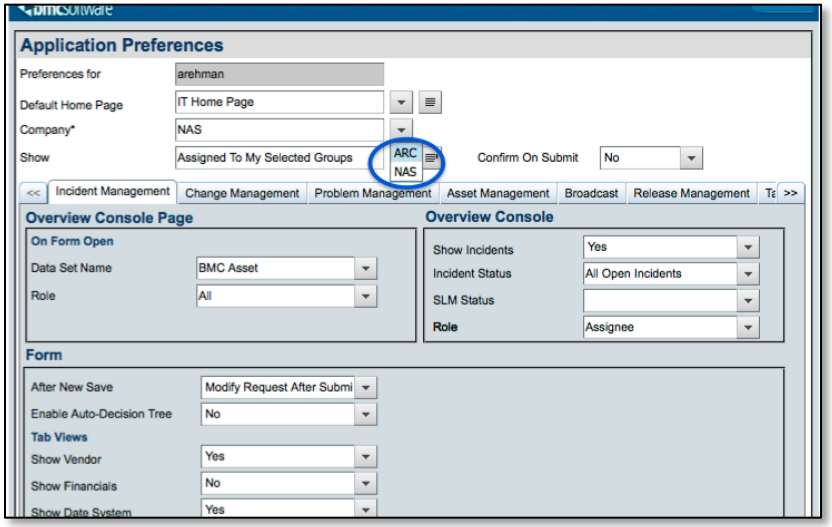
This diagram shows the configuration of a Pleiades Westmere node with the processor IDs labeled for each core. When users run jobs on Pleiades, SGI's Message Passing Toolkit (MPT) library automatically pins processes to contiguous cores. However, optimizing user scripts to keep the processes scattered instead of contiguous can improve job efficiency when a large-memory job leaves cores idle.

POC: Johnny Chang, johnny.chang@nasa.gov, (650) 604-4356, NASA Advanced Supercomputing Division, Computer Sciences Corp.

HECC Remedy Application and Expertise Leveraged to Support Ames' IT Directorate

- The HECC Tools team modified the Remedy application, used for incident tracking and other purposes, to support the trouble ticketing requirements of NASA Ames' Information Technology Directorate (Code I). The implementation went into production on August 7.
- With access to the modified Remedy version and new servers, Code I initially saved $150K, with ongoing annual savings of $25K. HECC will save on future server purchases—sharing half the cost with Code I—and gain additional Remedy technical support from Code I, when needed.
- Setup efforts included:
  - Defining Code I foundation data for support groups, ticket categorizations, users, and other information.
  - Integrating the NASA Enterprise Directory (NED) database for NASA people data, and customization of a multi-tenancy feature to share people data between Code I and HECC.
  - Setting up notification and workflow templates, user accounts, and user profiles.
- Future enhancements could include the capability to easily transfer tickets between the two organizations and implementation of additional HECC features into the Code I environment.

Mission Impact: By leveraging HECC's existing infrastructure and staffing expertise, two organizations can now be supported at minimal additional cost—resulting in benefits and savings to both organizations and laying the groundwork for hosting additional organizations.



Snapshot of screen showing Remedy's capability to host multiple organizations. This "multi-tenancy" feature allows each organization to have its own Remedy environment and unique users.

POC: Catherine Schulbach, Catherine.H.Schulbach@nasa.gov, (650) 604-3180, NASA Advanced Supercomputing Division

Maintenance Activities Successfully Completed During N258 Cooling Shutdown

- On August 2, the HECC Facilities team shut down the building N258 cooling systems to perform maintenance on the cooling tower, as part of a three-day scheduled downtime (see slide 8).
- The team coordinated with other HECC groups to complete several important maintenance activities. Work included:
  - Cleaning the cooling tower, including the silt buildup in the cooling tower sump. Cleaning this out reduces stress on pumps and motors, and allows the cooling tower to run more efficiently.
  - Cleaning the four 450-ton chillers to reduce particulates in the chilled water loop and maintain efficient water flow through the chilled water loop.
  - Completing system maintenance activities for compute servers, archive servers, license servers, and the NFS server migration.
- Accomplishing these maintenance tasks helps ensure the cooling tower remains operational until the new cooling tower construction is complete in summer 2015.

Mission Impact: Conducting regular maintenance on HECC infrastructure reduces the likelihood of unscheduled downtime that can impact users' ability to complete their science and engineering projects.

Photo of the NAS facility cooling tower, which provides 6 megawatts of cooling capacity for NASA's largest supercomputing facility.

POCs: Mark Tangney, mark.l.tangney@nasa.gov, (650) 604-4415, NASA Advanced Supercomputing (NAS) Division; Chris Buchanan, chris.buchanan@nasa.gov, (650) 604-4308, NAS Division, Computer Sciences Corp.

Facilities Team Completes Pump Repairs to Bring Facility Cooling Back to Full Capacity

- HECC Facilities staff coordinated with Ames Research Center (ARC) counterparts to complete repairs of two cooling tower pumps for building N258 that failed on July 12.
- The team worked with ARC engineers to expedite repairs and conduct a root cause analysis of the incident. Engineers worked through numerous problems, including:
  - De-installation of the two faulty pumps.
  - Manufacturing of replacement parts.
  - Re-installation and load-testing of the repaired pumps and motors.
  - Heating the two pump motors at specified temperatures to resolve an issue with them being "out of spec" for production.
- HECC staff coordinated cleaning of the cooling tower and four 450-ton chillers while repairs were being completed (see slide 7), and ensured all cooling system components were ready for production before bringing cooling and power back up to full capacity.

Mission Impact: HECC experts' rapid response and coordination efforts expedited repairs to critical supercomputing facility infrastructure, and enabled the Pleiades supercomputer to return to full operation for NASA scientific and engineering users.

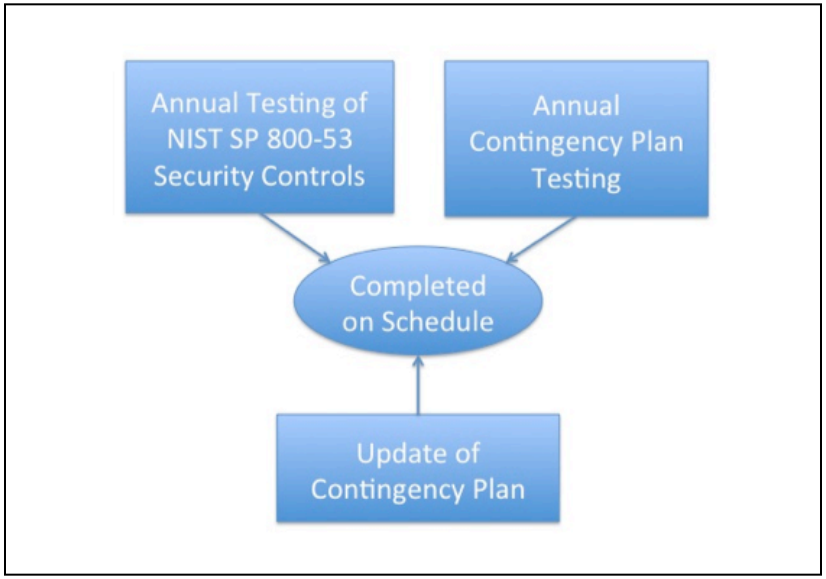
Photo showing the four cooling tower pumps at the NAS facility, following the repairs of pumps 2 and 3 (in the middle).

POCs: Mark Tangney, mark.l.tangney@nasa.gov, (650) 604-4415, NASA Advanced Supercomputing (NAS) Division; Chris Buchanan, chris.buchanan@nasa.gov, (650) 604-4308, NAS Division, Computer Sciences Corp.

Annual Control and Contingency Testing Activity Completed by July 30 Deadline

- An important compliance requirement associated with NASA security plans is the testing of a significant portion of the National Institute of Standards and Technology (NIST) SP 800-53 Security and Privacy Controls and Contingency Planning.
- HECC security staff completed many months of control testing, and all 133 controls passed. They also performed an annual review of the NAS contingency plan and made minor updates.
- HECC also completed a functional review test, in which the project's teams showed they could continue to keep all high-end systems running at full capacity under the conditions of this year's test scenario: exposure to a virulent disease that required some staff work from home.
- All required tasks were performed by the July 30 deadline and results were uploaded to the agency repository for security plans and associated documents.

Mission Impact: Successful completion of NASA's annual control and contingency plan tests will help the HECC project maintain its authorization to operate agency supercomputing resources.



High-End Computing Capability Project security experts successfully completed all of the annual security testing required by the National Institute of Standards and Technology.

POC: Thomas Hinke, thomas.h.hinke@nasa.gov, (650) 604-3662, NASA Advanced Supercomputing Division

Pleiades Enables New Discovery in Nonlinear Slosh Dynamics for Propellant Tanks *

- Researchers at Marshall Space Flight Center (MSFC) performed multi-phase CFD simulations on Pleiades to address the challenge of accurately predicting smooth-wall propellant tank slosh dynamics, which can critically affect launch and space vehicle stability.
- The CFD simulations were first validated against experimental data for linear slosh damping within various tank sizes and showed very good agreement.
- Simulations show that slosh damping is a function of slosh amplitude.
  - Researchers discovered that once the slosh amplitude reaches a critical value, the damping ratio increases linearly with the slosh amplitude.
  - This discovery could lead to significant savings in launch vehicle development by reducing the number and size of slosh baffles needed in liquid propellant tanks.
- Very fine grid resolutions are needed to capture the thin boundary profile of propellant slosh waves and associated low fluid damping. The simulations would not be possible without the use of Pleiades to solve the complex, multi-phase flow problems.

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

Mission Impact: The Pleiades supercomputer's highly parallel processing capabilities enabled a discovery that could help engineers to redesign liquid propellant tanks, which would lead to significant savings in launch vehicle development time and costs.

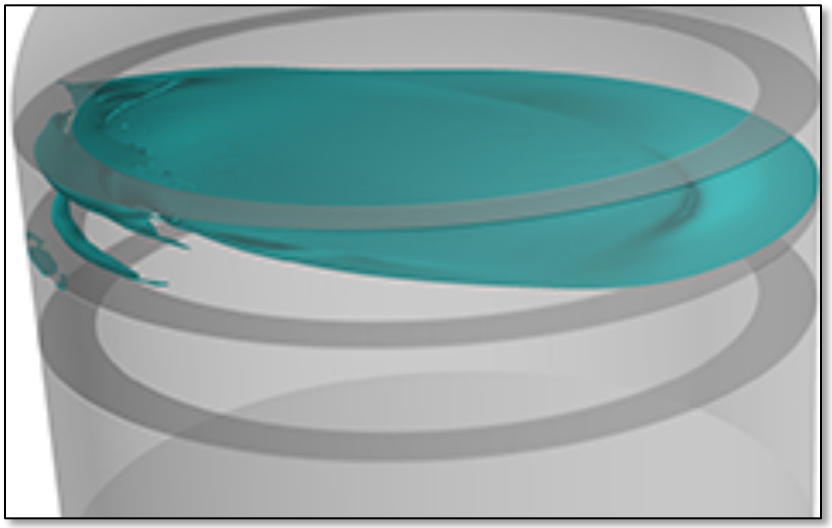


Image from a CFD simulation of slosh dynamics, showing free surface waves inside a propellant tank with baffles. Submerged gas bubbles near the baffle surface show that nonlinear damping physics prevail in this case, even under a small slosh amplitude. Consideration of nonlinear slosh damping can lessen the number and size of slosh baffles required.

POCs: Jeff West, jeffrey.s.west@nasa.gov, (256) 544.6309; H. Q. Yang, hong.q.yang@nasa.gov, (256) 544.8978, NASA Marshall Space Flight Center

Simulations Run on Pleiades Reveal Clues to the Interior of Venus *

- Researchers at NASA's Jet Propulsion Laboratory (JPL) ran long-duration simulations on Pleiades to verify spacecraft observations of volcanic plumes and surface topology on Venus.
- The simulations enabled the JPL team to explore many parameters, including temperature-dependent viscosity, Rayleigh number, interior viscosity, interior temperature differences, internal heating, and free-slip and no-slip top and bottom boundaries. Among the team's findings:
  - The mantle of Venus might not be in thermal equilibrium; rather, it may be heating up over time.
  - Given the predicted mass flux from plumes and the amount of water estimated to exist in Venus' interior, plume volcanism (which releases volatile gases) could provide the observed concentrations of water vapor in the planet's atmosphere.
  - Water in the mantle facilitates melting and volcanism. If volcanism occurs only over plumes, it would suggest that water brought up from the lower mantle by plumes is needed to cause wet melting.
- Pleiades enabled the JPL model to run for long durations to reach steady state, with each simulation using many processors in parallel.

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

Mission Impact: Long-duration simulations, enabled by the Pleiades supercomputer, allow scientists to evaluate a wide range of parameters to study the internal dynamics of Venus and other planets and improve our understanding of the planets, satellites and smaller bodies in the solar system.

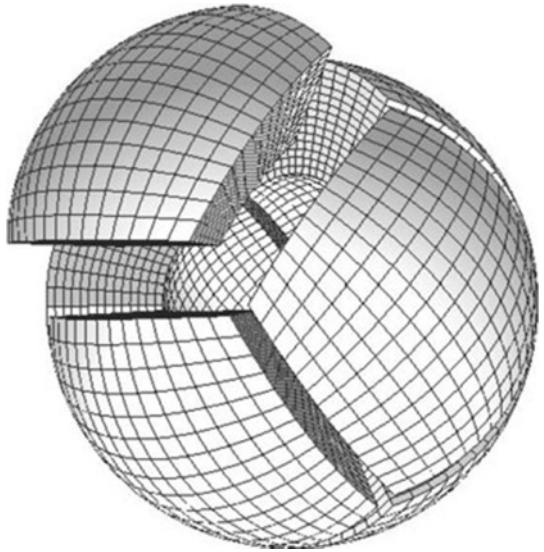


Diagram of a cube-sphere 3D grid used for a numerical model of the interior of Venus. The model was built using OEDIPUS, a code developed specifically to study the internal dynamics of planets.

POC: Suzanne Smrekar, suzanne.e.smrekar@jpl.nasa.gov, (818) 354-4192, NASA Jet Propulsion Laboratory

HECC Facility Hosts Several Visitors and Tours in August 2014

- HECC hosted 9 tour groups in August; guests learned about the agency-wide missions being supported by Pleiades, and viewed the QuAIL system.
- NOTE: Due to facility outages and the hyperwall computer system upgrade, many tours have been postponed until the hyperwall is returned to production.
- Visitors this month included:
  - Larry James, JPL deputy director, was given an overview and tour of the NAS facility by Piyush Mehrotra.
  - Grace Hu, chief budget examiner, Office of Management and Budget for NASA Science; and Jens Feeley, deputy director, Strategic Integration and Management Division, Science Mission Directorate at NASA Headquarters, were also given an overview and tour by Piyush Mehrotra;
  - Center Director Pete Worden invited all ARC summer interns to visit the quantum computer; 143 students from the 2014 Ames Summer Internship Program heard a quantum computing technical lecture by Rupak Biswas and Piyush Mehrotra, followed by a tour of the quantum computer room.

HECC staff organized three large group tours for Ames summer interns in August. Participants enjoyed a technical lecture and toured the quantum computer room. Pictured above, NAS Division Chief Piyush Mehrotra speaking to a group of interns.

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

Papers and Presentations

- "**Geospatial Spreadsheets with Microscale Air Quality Visualization and Synchronization for Supporting Multiple-Scenario Visual Collaboration**," S. M. An, H.-Y. Lee, B. Kim, J.-H. Eum, J.-H. Woo, International Journal of Geographical Information Science, August 8, 2014. *
  http://www.tandfonline.com/doi/abs/10.1080/13658816.2014.938077
- "**Time-Distance Helioseismology of Two Realistic Sunspot Simulations**," K. DeGrave, J. Jackiewicz, M. Rempel, arXiv:1408.2262 [astro-ph.SR], August 10, 2014. *
  http://arxiv.org/abs/1408.2262
- "**Handy's Harbinger**," D. Schwenke, presented at the 248th American Chemical Society National Meeting, San Francisco, CA, August 10-14, 2014.
  http://abstracts.acs.org/chem/248nm/program/view.php?obj_id=271207
- "**Simulations of Boreal Summer Interseasonal Oscillations with the Climate Forecast System, version 2, over India and the Western Pacific: Role of Air-Sea Coupling**," R. P. Shukla, J. Zhu, Atmosphere-Ocean, August 12, 2014. *
  http://www.tandfonline.com/doi/abs/10.1080/07055900.2014.939575
- "**Radial Velocity Observations and Light Curve Noise Modeling Confirm that Kepler-91b is a Giant Planet Orbiting a Giant Star**," T. Barclay, et al., arXiv:1408.3149 [astro-ph.EP], August 13, 2014. *
  http://arxiv.org/abs/1408.3149

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

Papers and Presentations (cont.)

- "**The Migration of Gap-Opening Planets is not Locked to Viscous Disk Evolution**," P. C. Duffell, Z. Haiman, A. I. MacFadyen, D. J. D'Orazio, B. D. Farris, The Astrophysical Journal Letters, vol. 792, no. 1, August 14, 2014. * *http://iopscience.iop.org/2041-8205/792/1/L10*
- "**Ion Energization and Transport Associated with Magnetic Dipolarizations**," Q. Pan, M. Ashour-Abdalla, R. J. Walker, M. El-Alaoui, Geophysical Research Letters (Early View), August 22, 2014. * *http://onlinelibrary.wiley.com/doi/10.1002/2014GL061209/full*
- "**NASA Embarks on the Quantum Computing Path**," R. Biswas, Air Combat Command's (ACC) West Coast Air Superiority Innovation Summit, August 27, 2014.

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

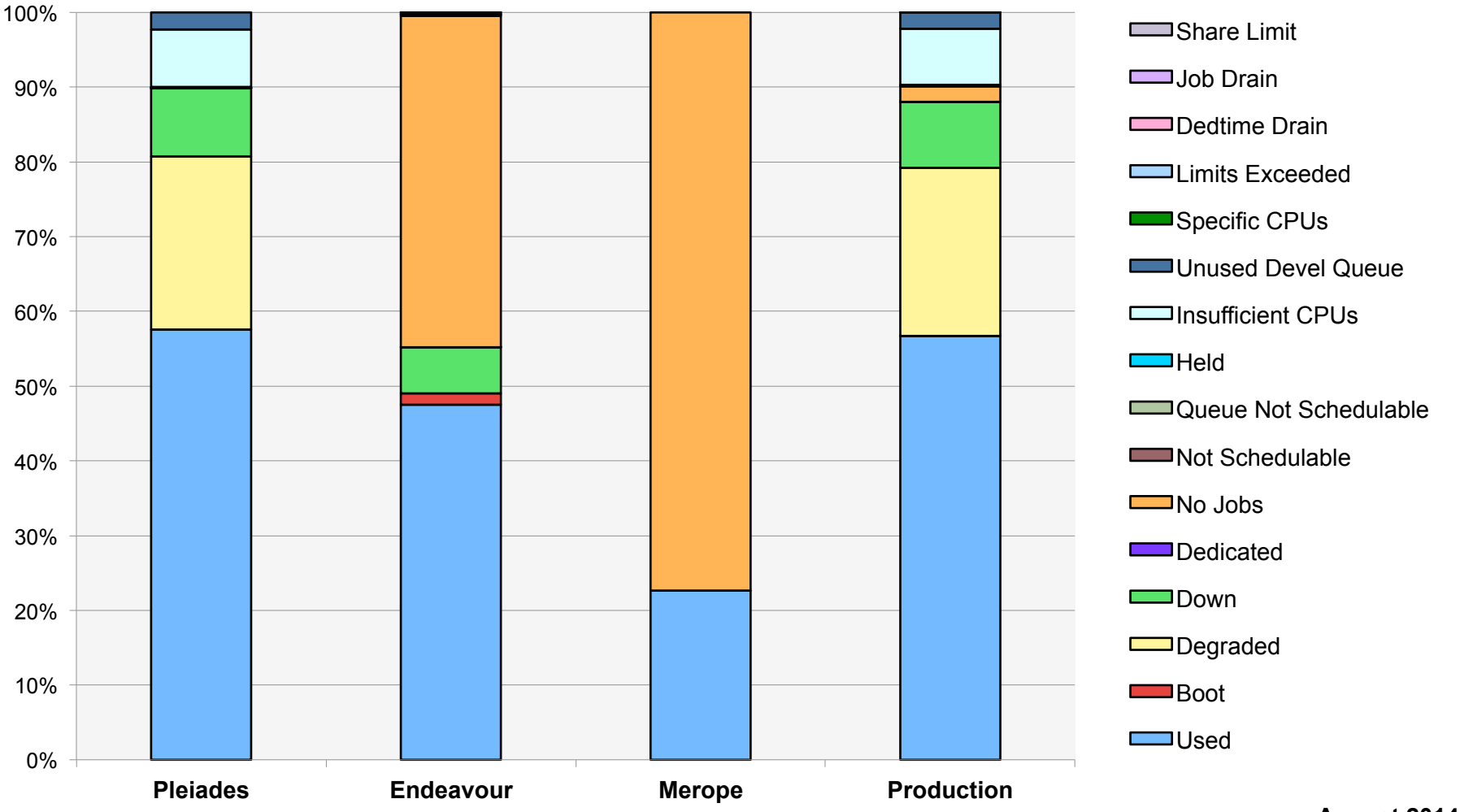
News and Events

- **NASA Picks Top Earth Data Challenge Ideas, Opens Call for Climate Apps**, *NASA Press Release*, August 22, 2014—NASA has selected four ideas from the public for innovative uses of climate projections and Earth-observing satellite data from the Open NASA Earth Exchange (OpenNEX). The agency also has announced a follow-on challenge with awards of $50,000 to build climate applications based on OpenNEX data on the Amazon cloud computing platform.
  http://www.nasa.gov/press/2014/august/nasa-picks-top-earth-data-challenge-ideas-opens-call-for-climate-apps

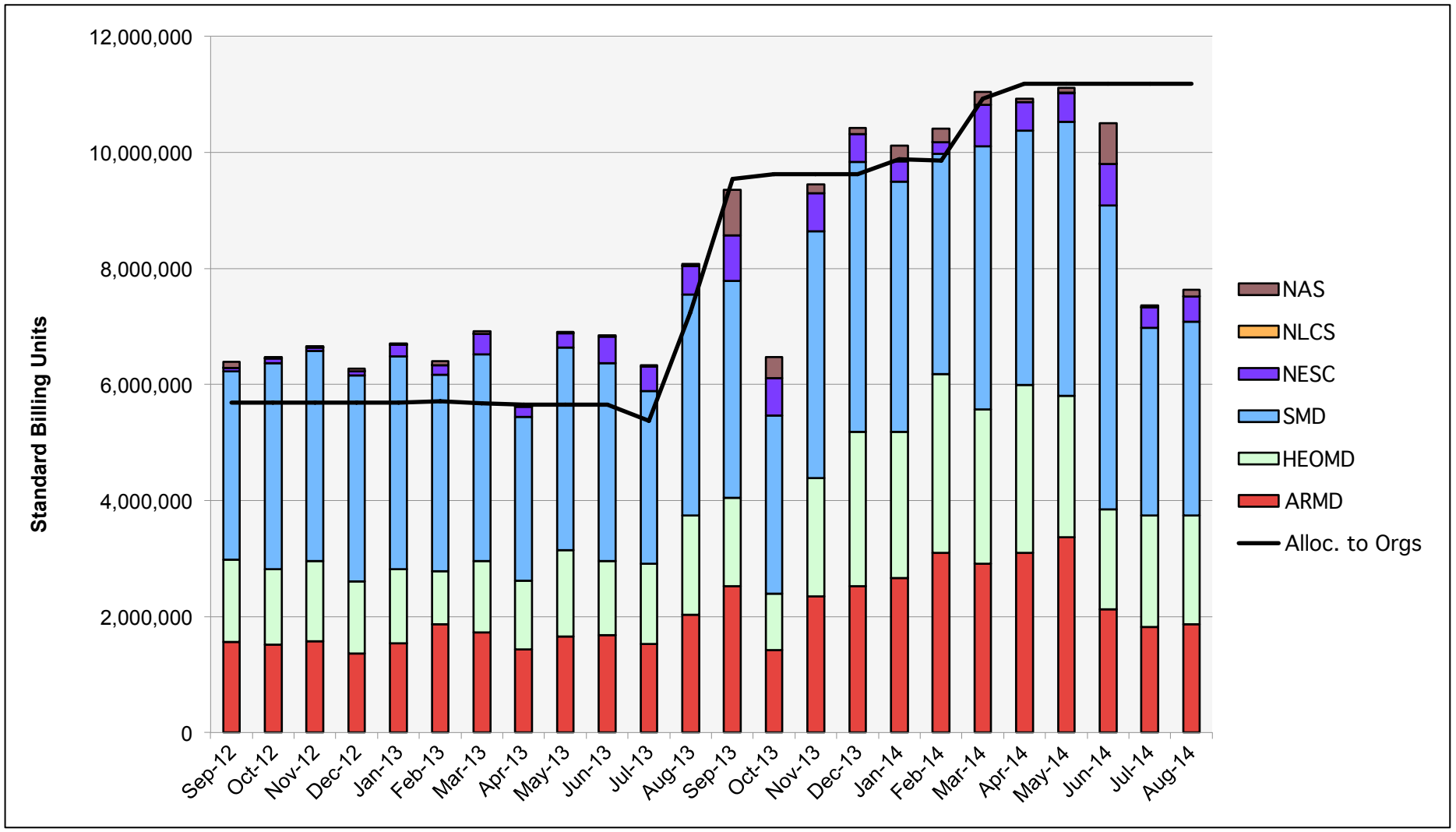
Phi-based Systems

- **Background:**
  Two Xeon Phi-based systems are being utilized as path-finding resources to determine whether the Many Integrated Core (MIC) Architecture is cost effective for NASA's computational requirements.
  - Maia is a 128-node SGI system with two Intel Xeon Phi accelerator cards in each node.
  - Mira is a 64-node Cray system with two Intel Xeon Phi accelerator cards in each node.
- **Status**
  - Both Maia and Mira were offline for much of the month due to the cooling pump issue at the main NAS facility. Maia was brought back online in mid-August, after the cooling pumps were restored.
  - Two HECC staff members attended an Intel "dungeon" (customer-focused lab) in Hillsboro, Oregon, along with several staff members from other NASA centers. The event focused on application performance optimization for both the current and next-generation Xeon Phi platforms.
- **Upcoming Activities for September**
  - Maia: The system is available for user testing.
  - Mira: The "NASification" process will most likely continue for a few more weeks.

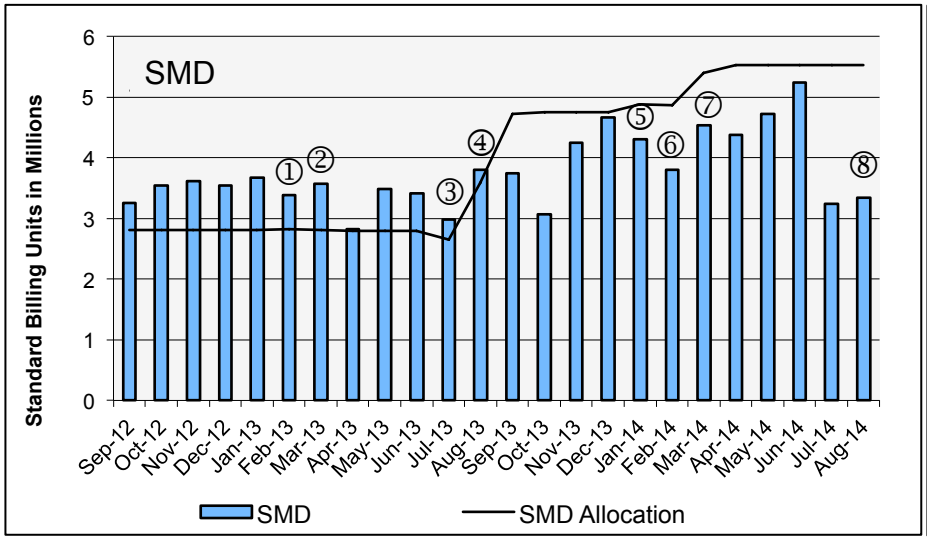
HECC Utilization

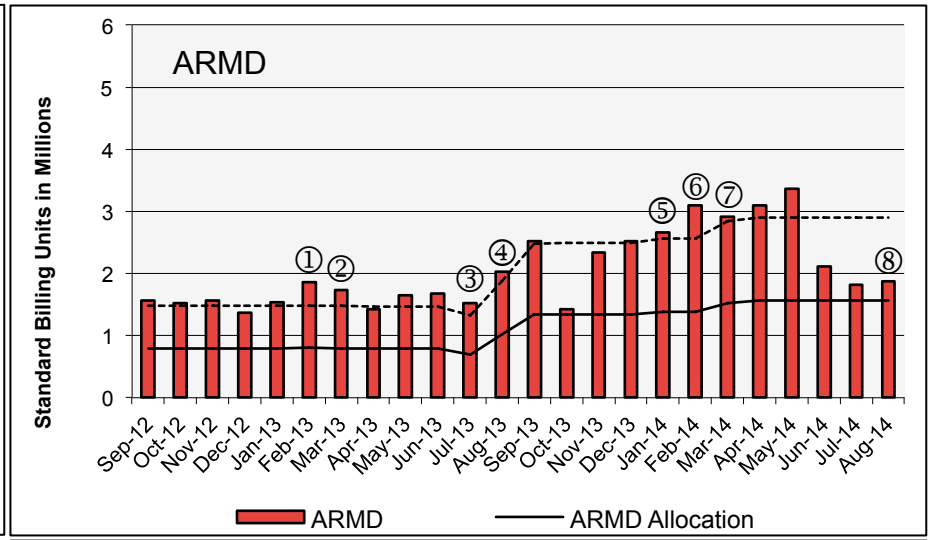


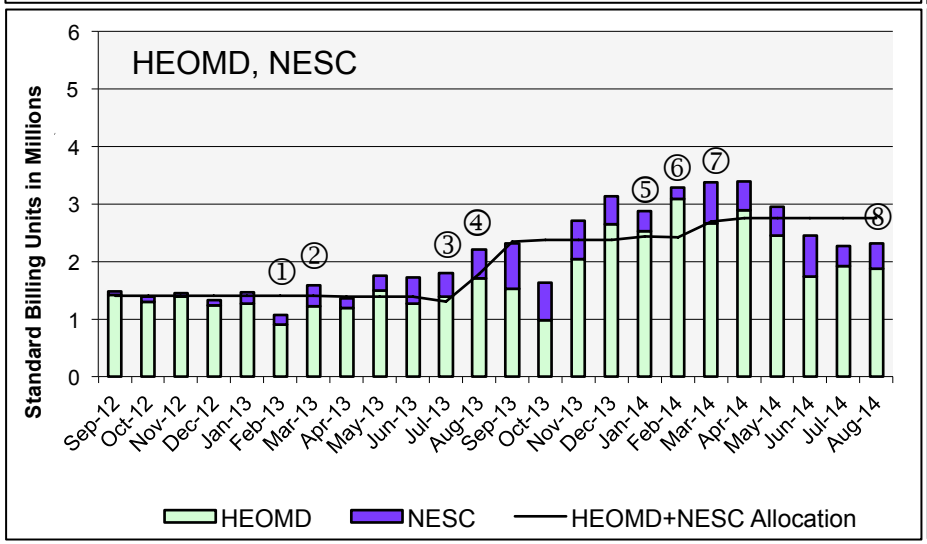
HECC Utilization Normalized to 30-Day Month



HECC Utilization Normalized to 30-Day Month

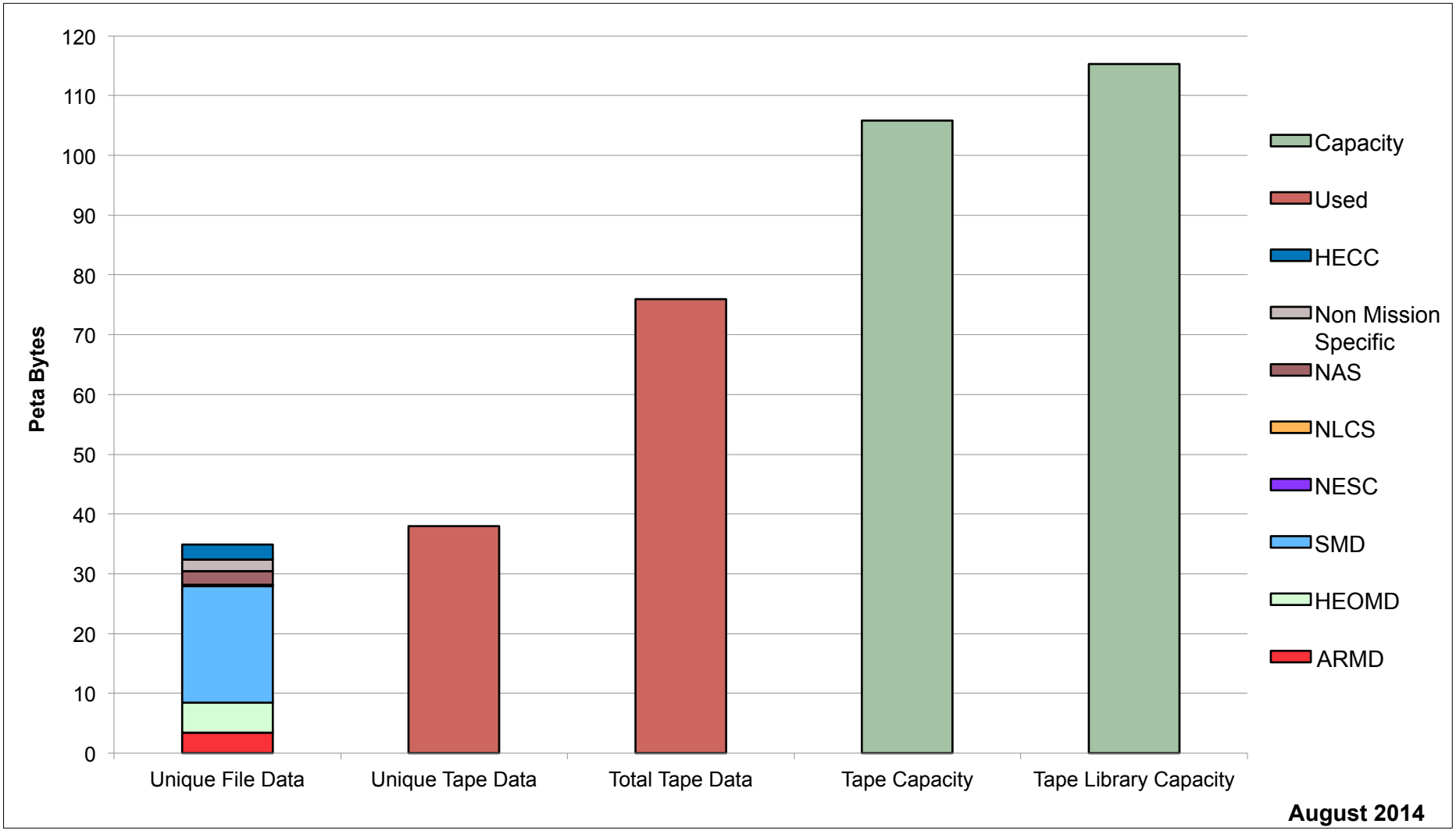






① Columbia 21, 23, and 24 retired, Endeavour 2 added
② Columbia 22 retired; Endeavour 1 added
③ 32 Harpertown Racks retired
④ 32 Harpertown Racks retired; 46 Ivy Bridge Racks added
⑤ 6 Ivy Bridge Racks added; 20 Nehalem and 12 Westmere Racks Retired
⑥ 8 Ivy Bridge Racks added mid-Feb; 8 additional Ivy Bridge Racks late Feb.
⑦ 4 Ivy Bridge Racks added mid-March
⑧ 8 Westmere Racks added to Merope

Tape Archive Status



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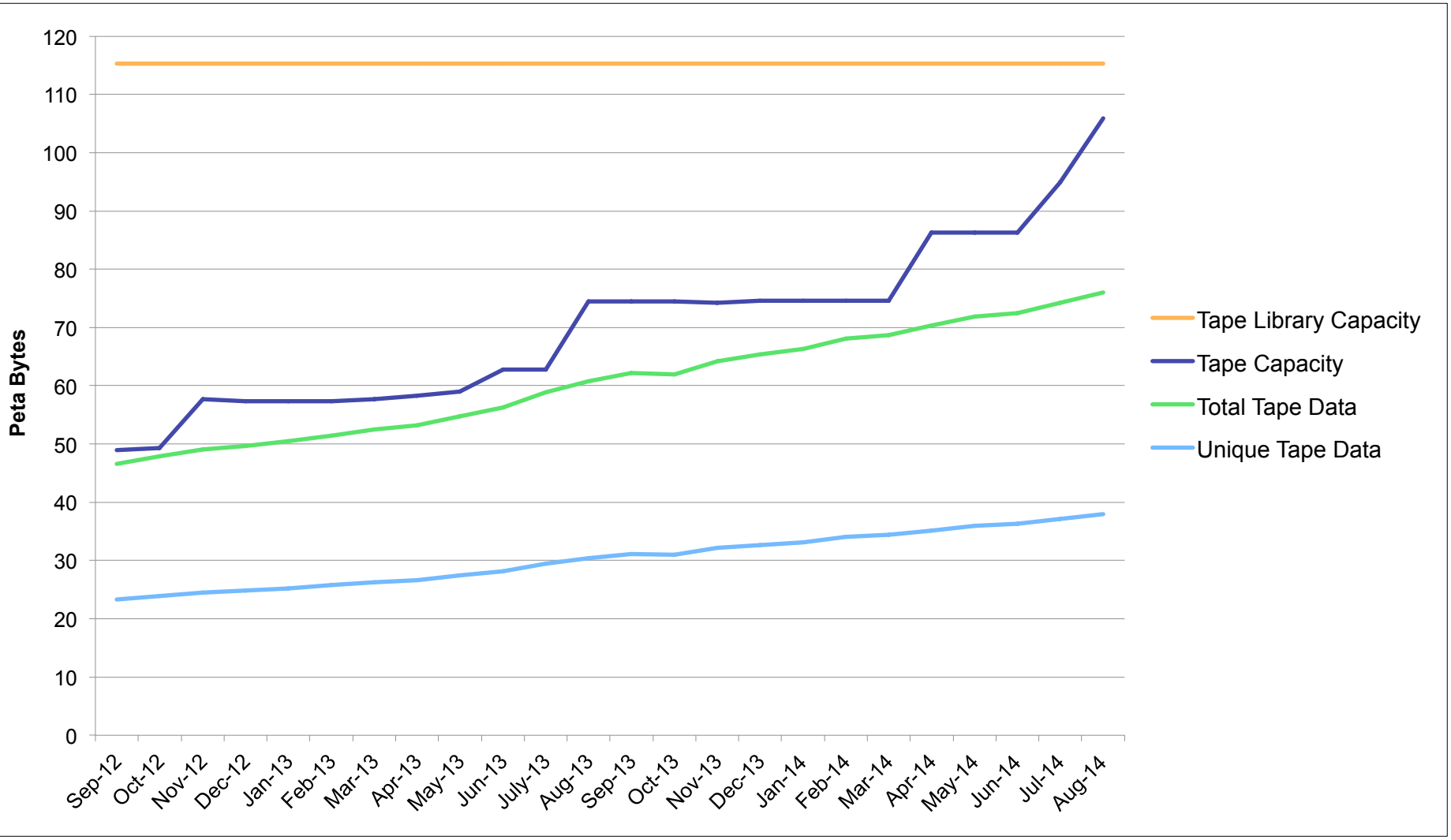
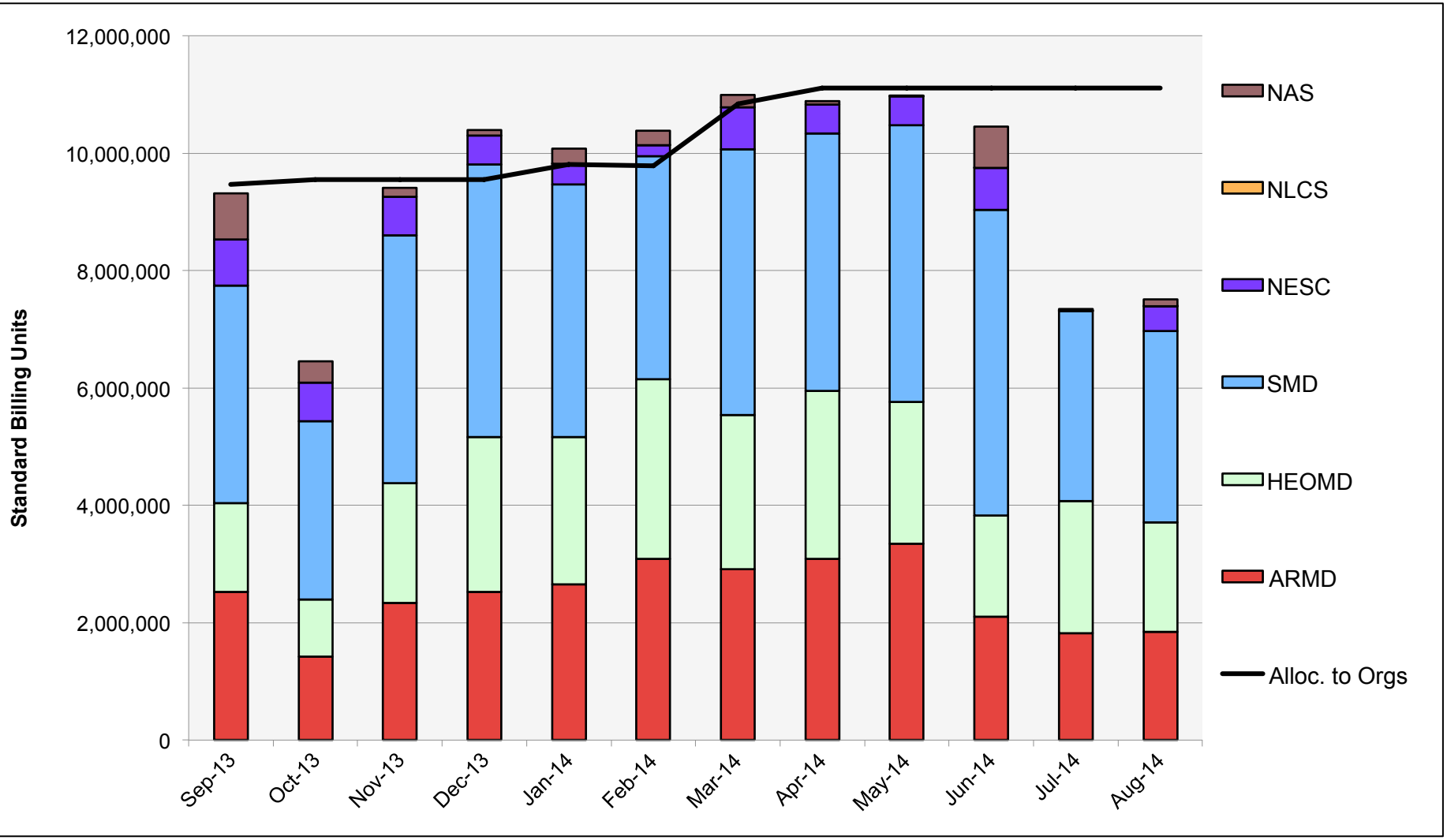
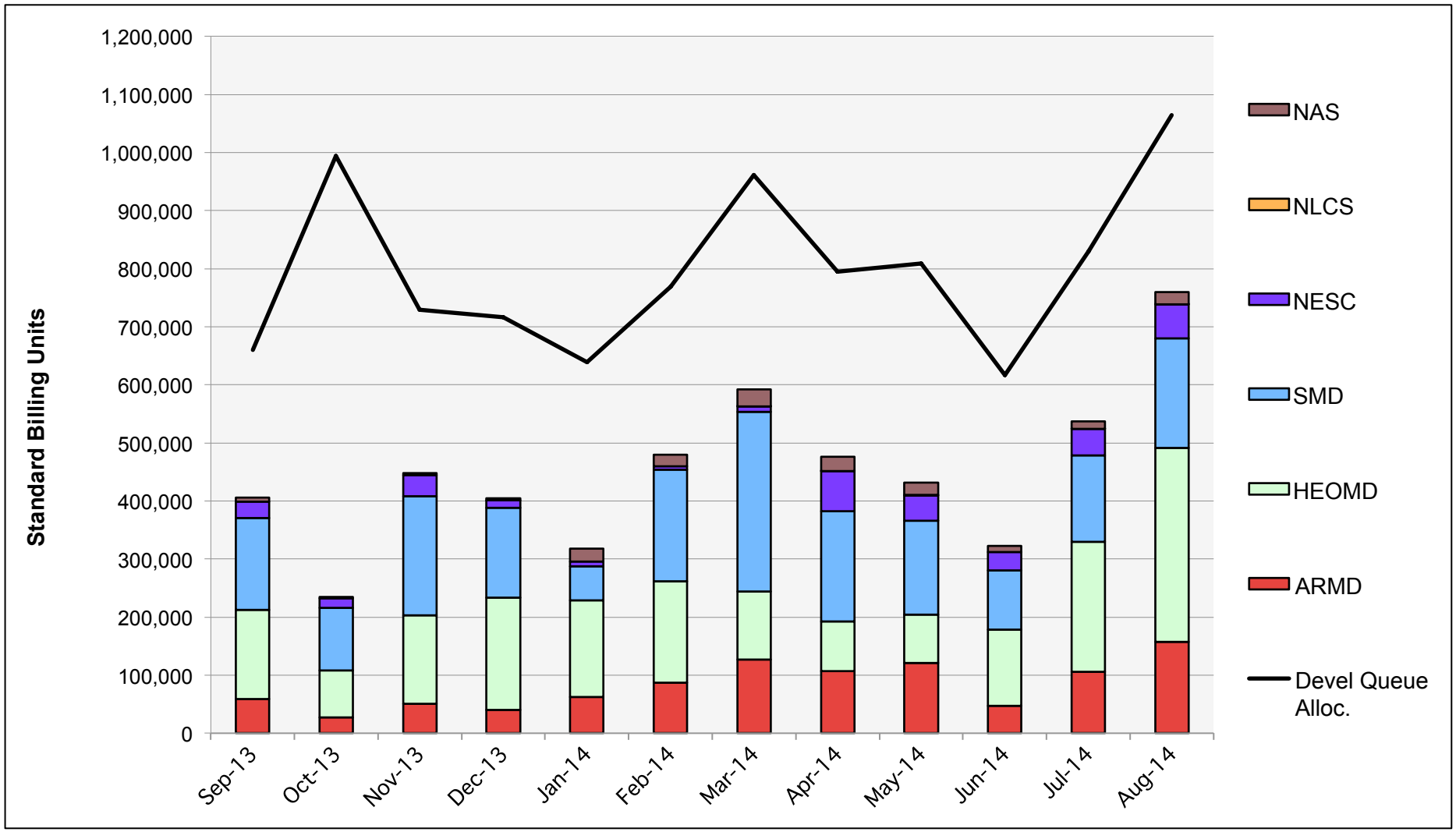


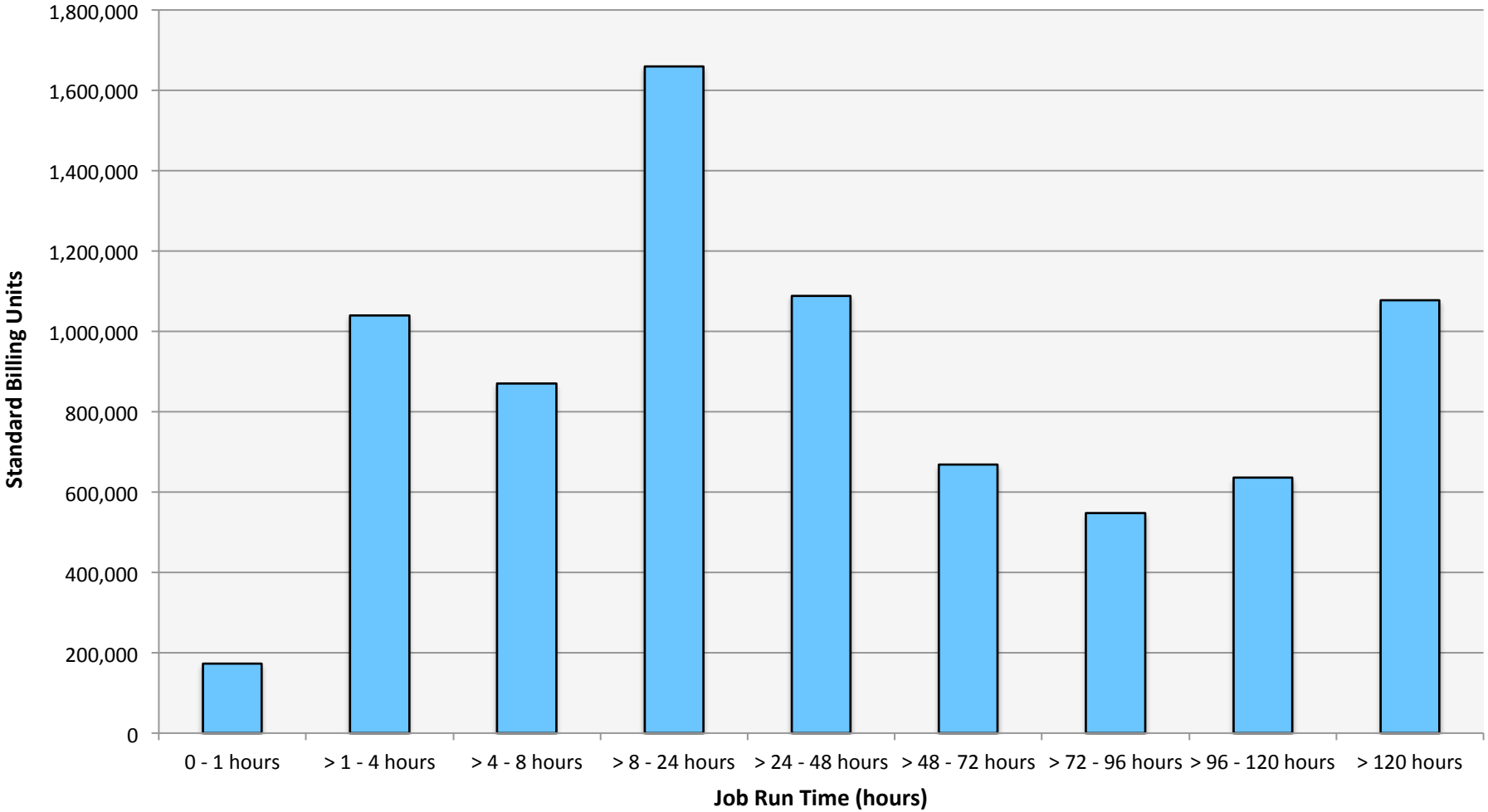
Pleiades:
SBUs Reported, Normalized to 30-Day Month



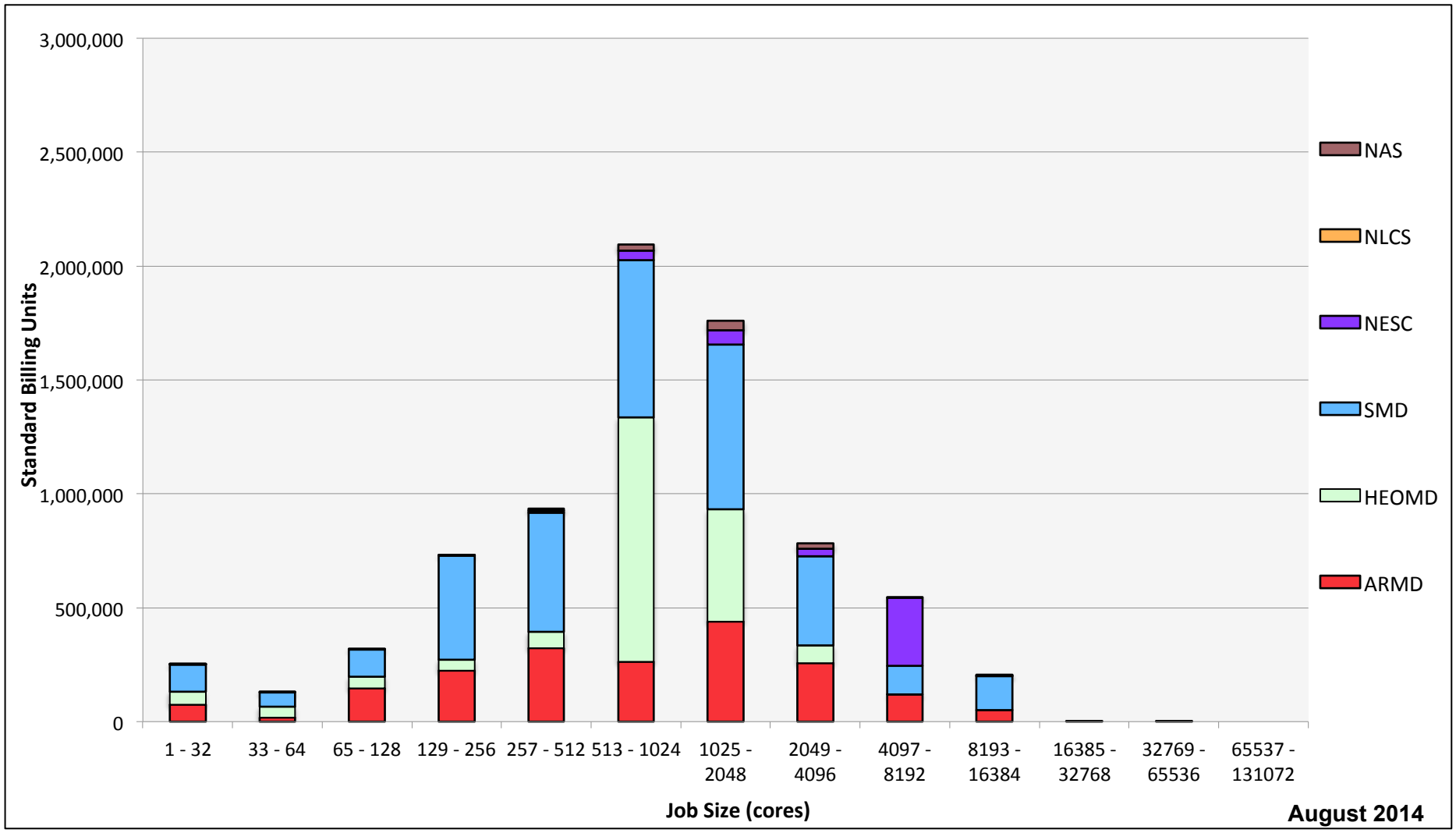
Pleiades:
Devel Queue Utilization



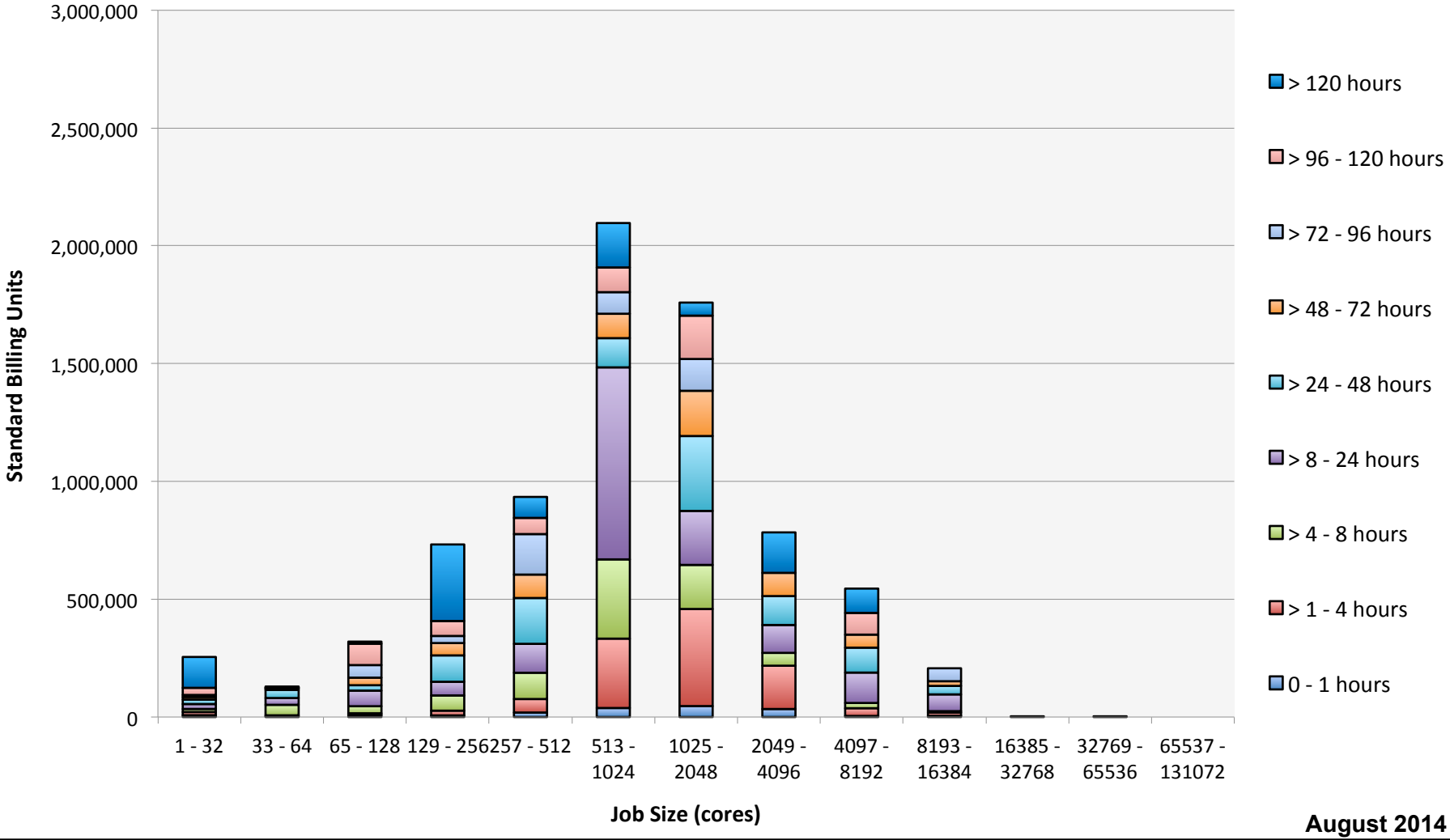
Pleiades:
Monthly Utilization by Job Length



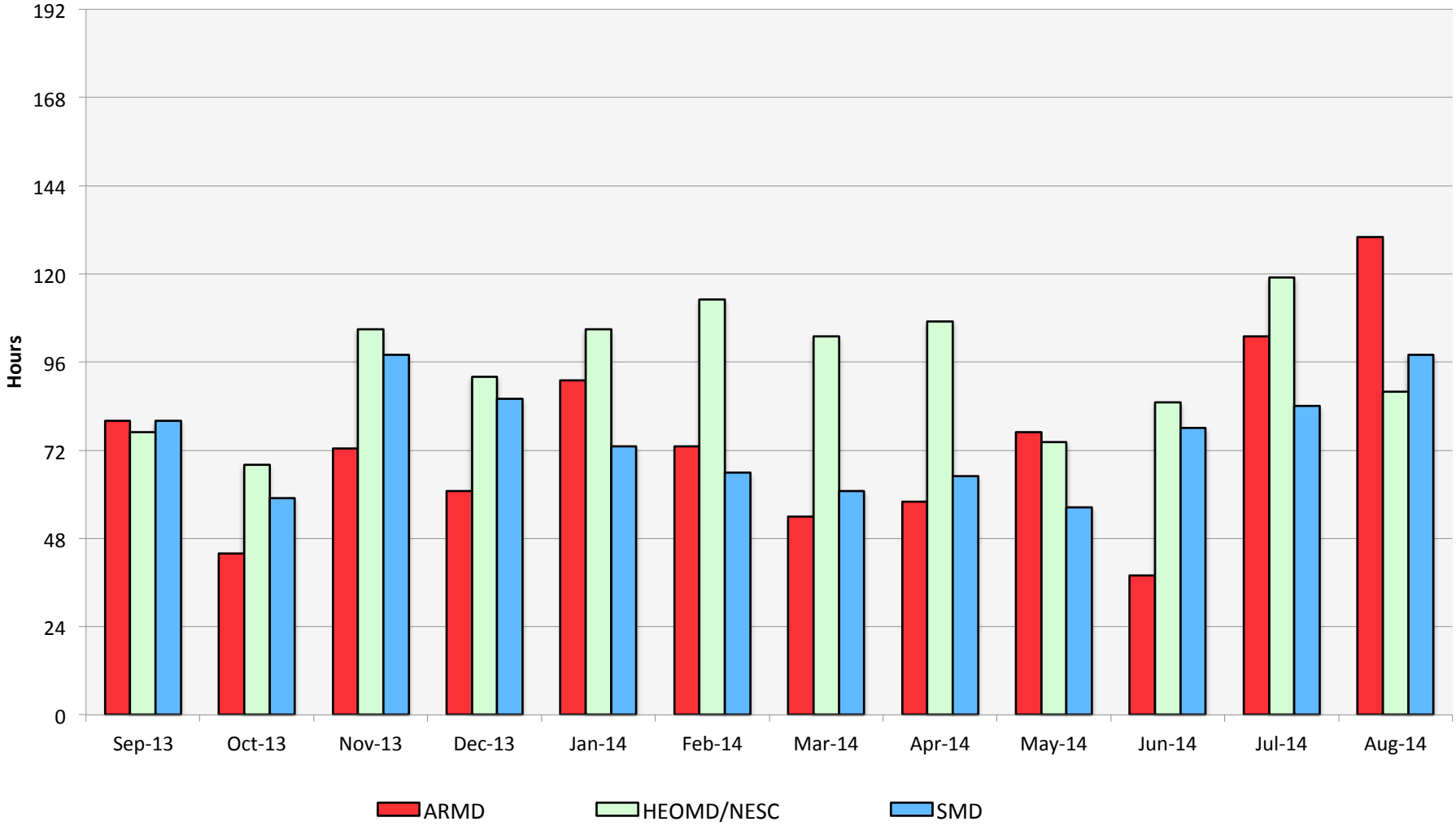
Pleiades:
Monthly Utilization by Size and Mission



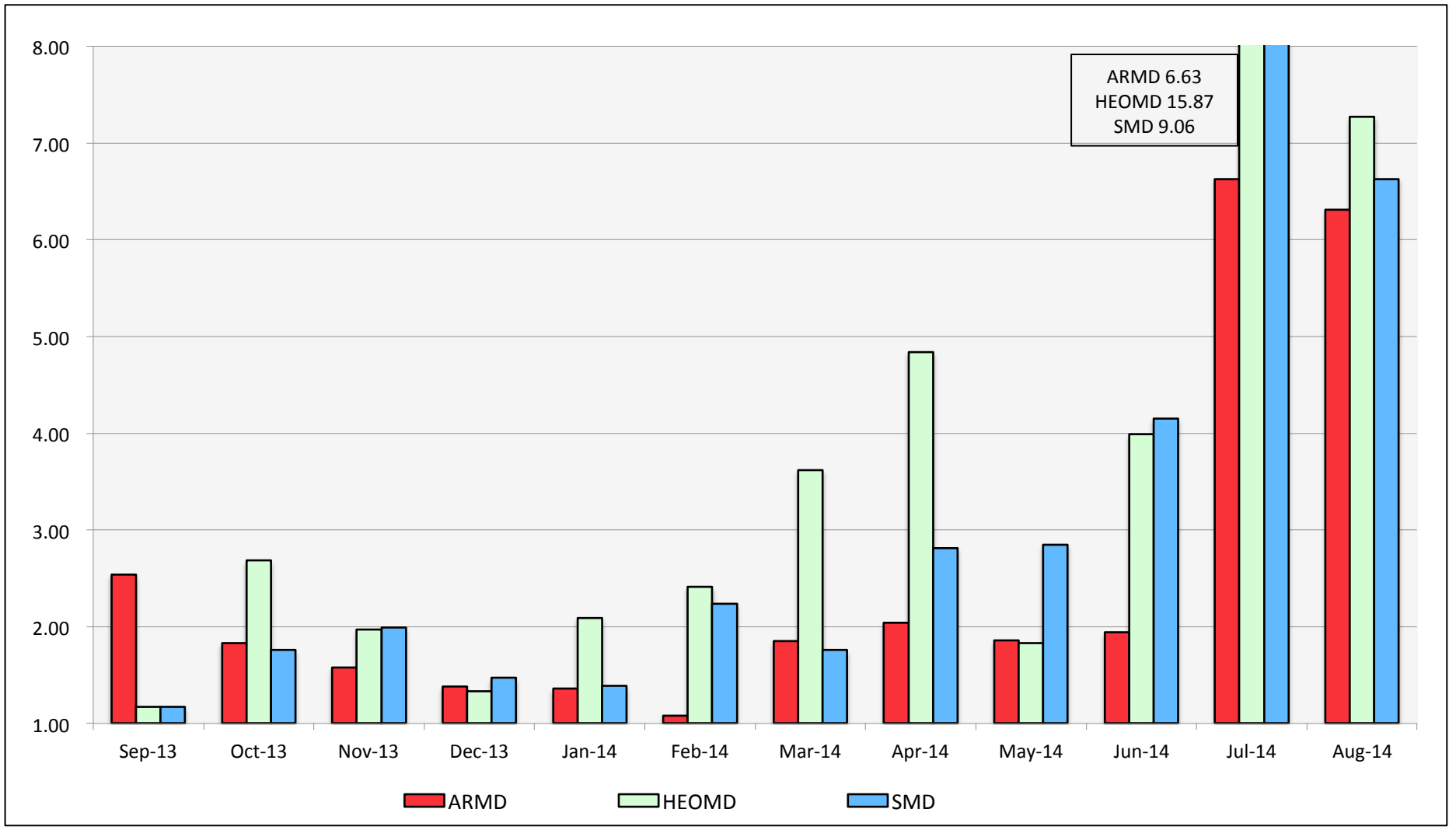
Pleiades:
Monthly Utilization by Size and Length



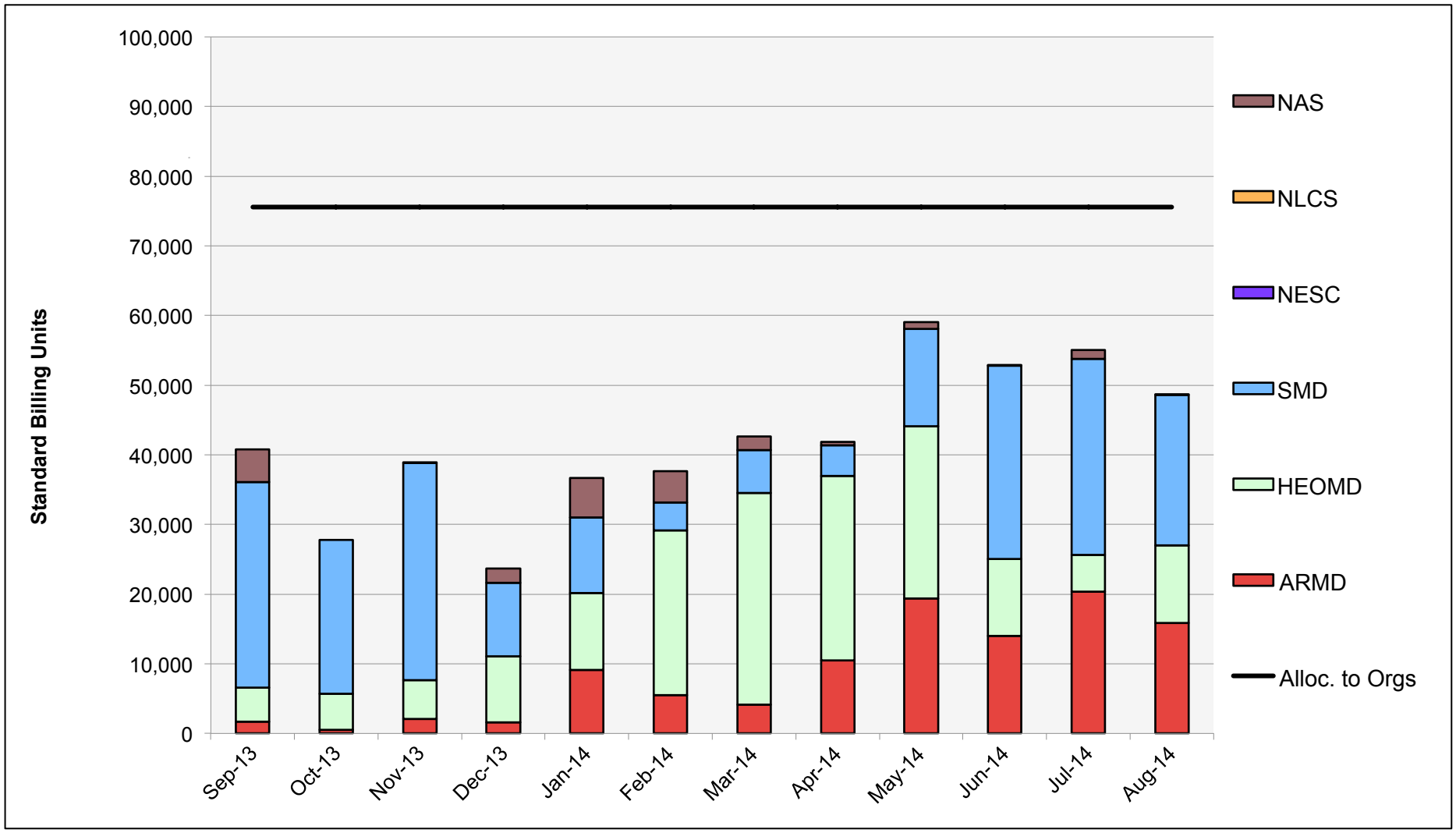
Pleiades:
Average Time to Clear All Jobs



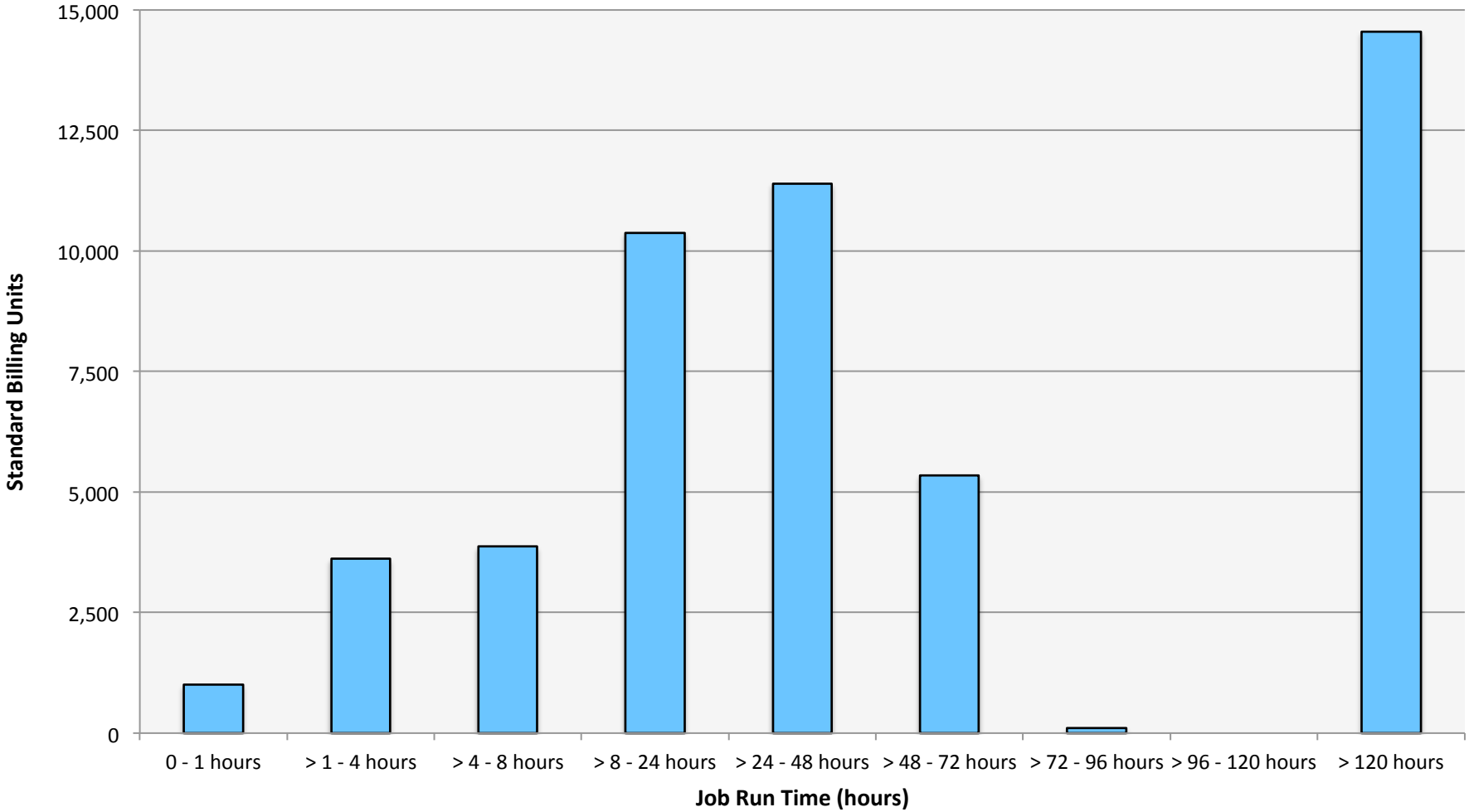
Pleiades:
Average Expansion Factor



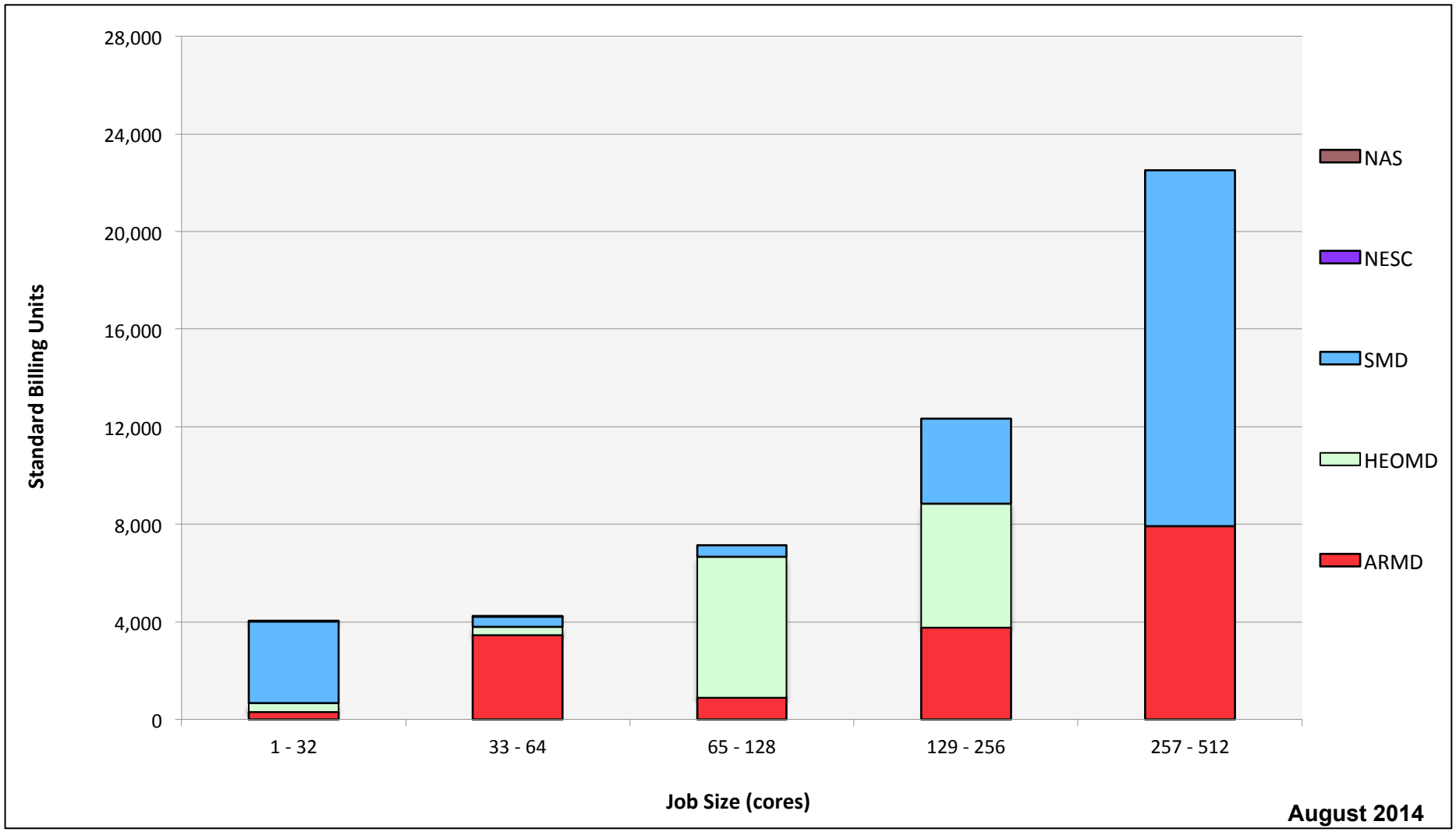
Endeavour:
SBUs Reported, Normalized to 30-Day Month



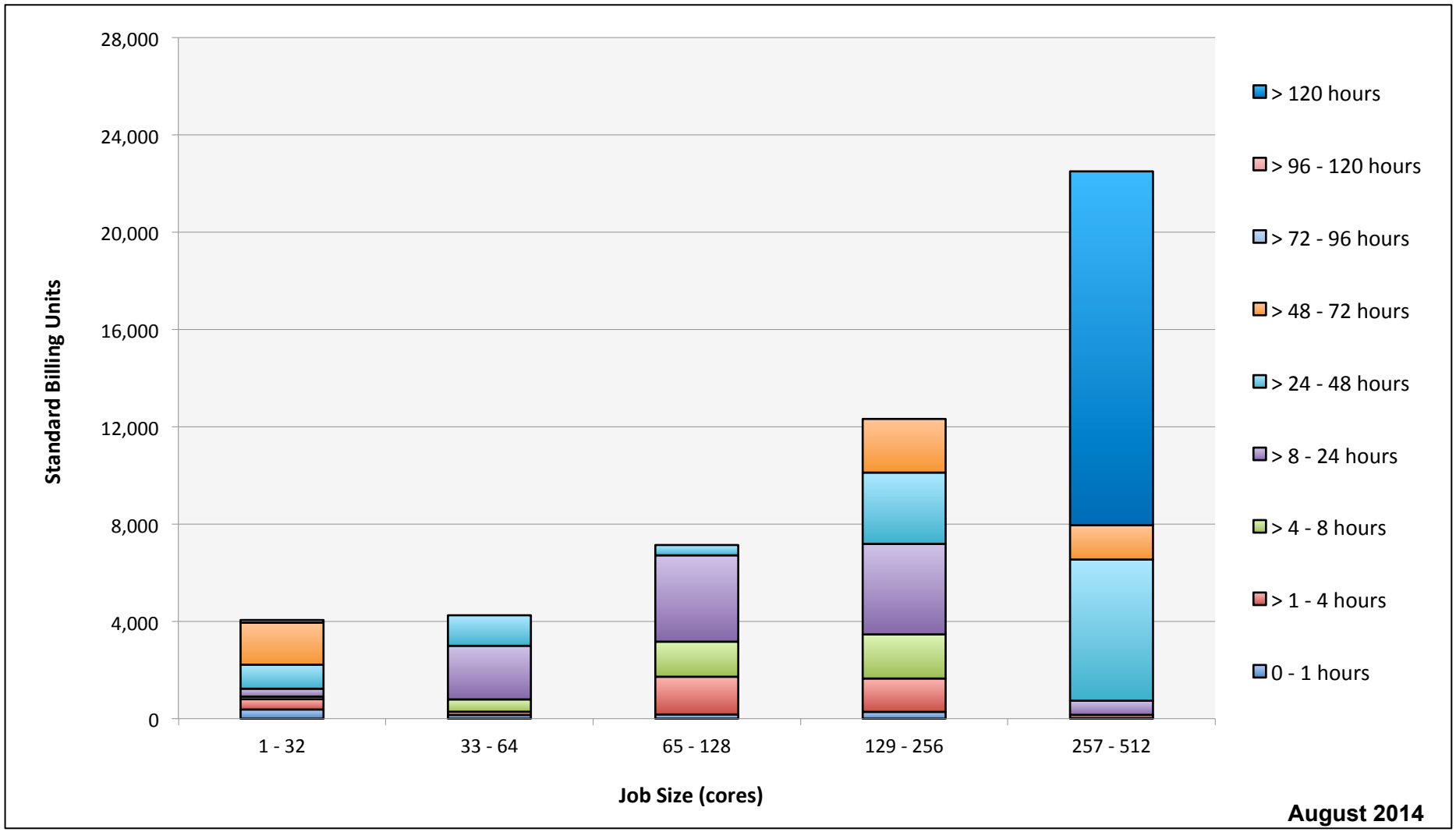
Endeavour:
Monthly Utilization by Job Length



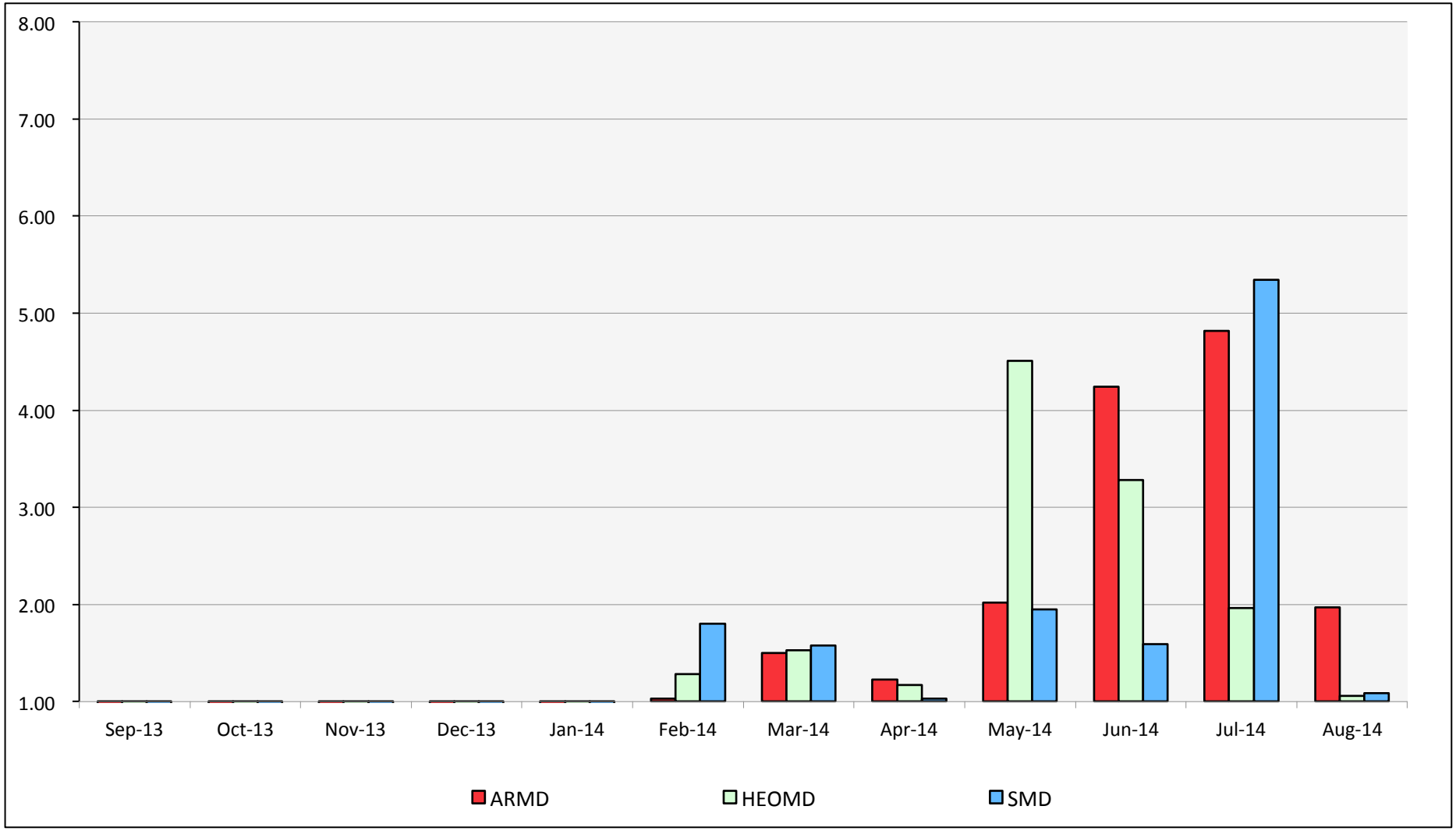
Endeavour:
Monthly Utilization by Size and Mission



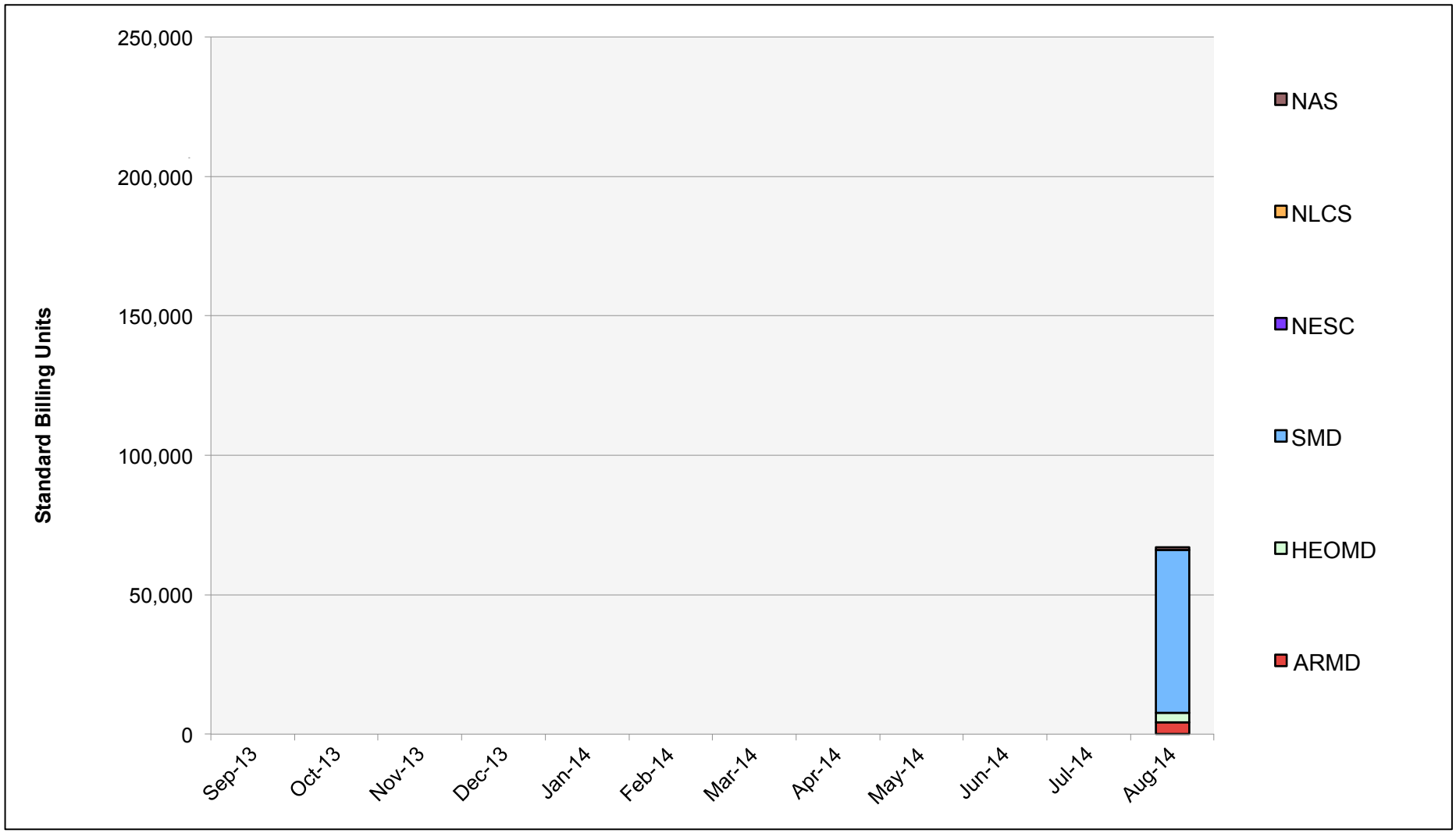
Endeavour:
Monthly Utilization by Size and Length



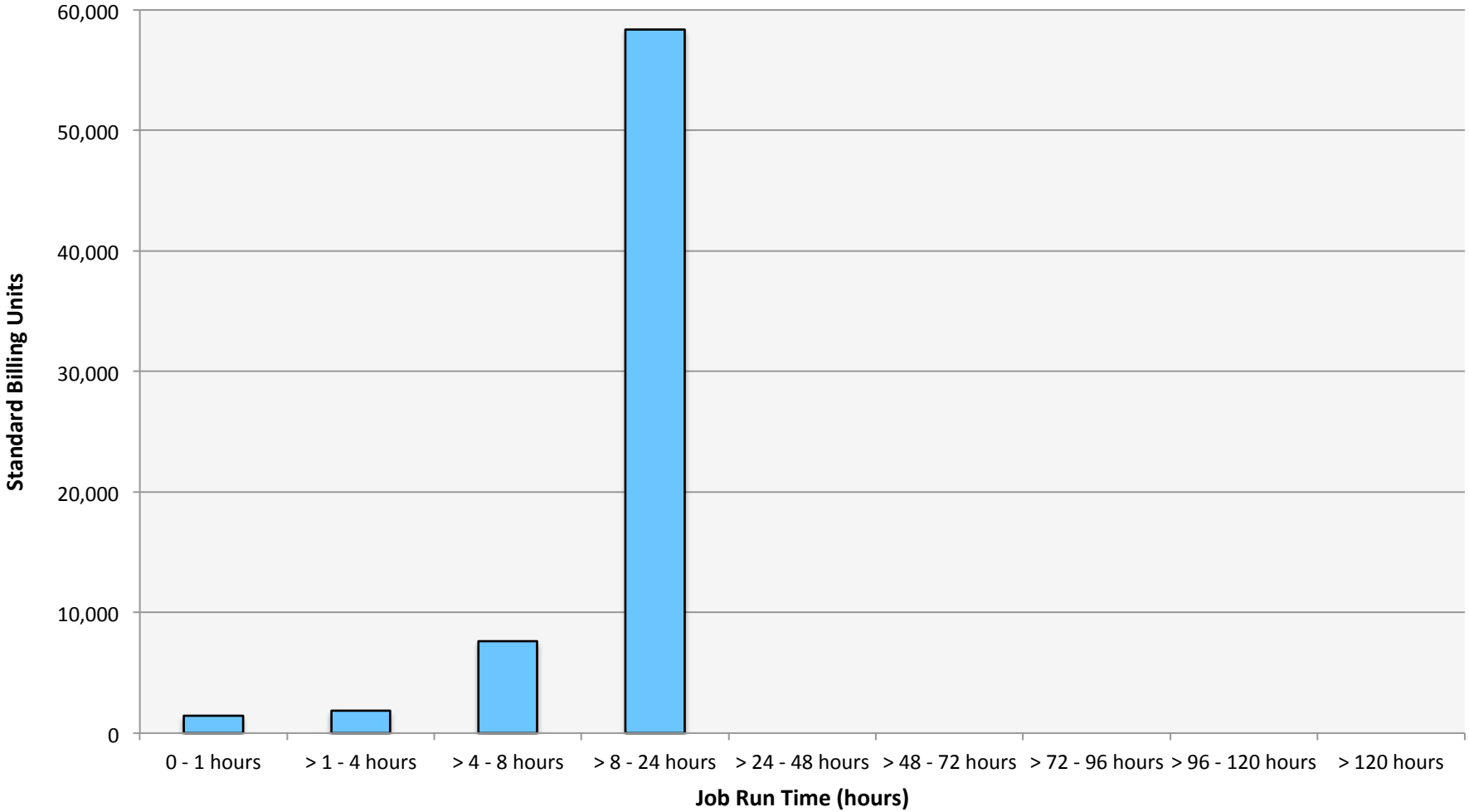
Endeavour:
Average Expansion Factor



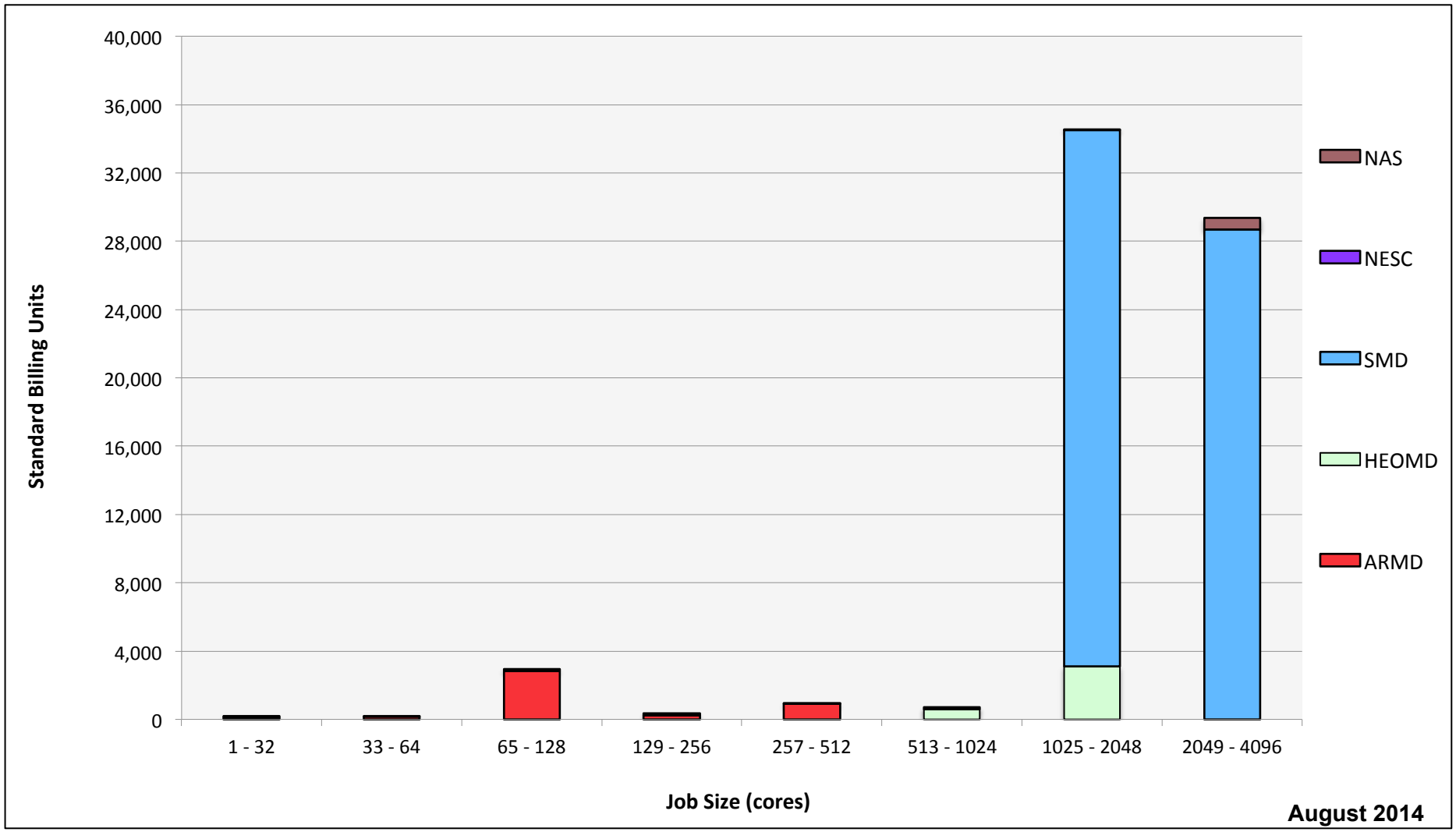
Merope:
SBUs Reported, Normalized to 30-Day Month



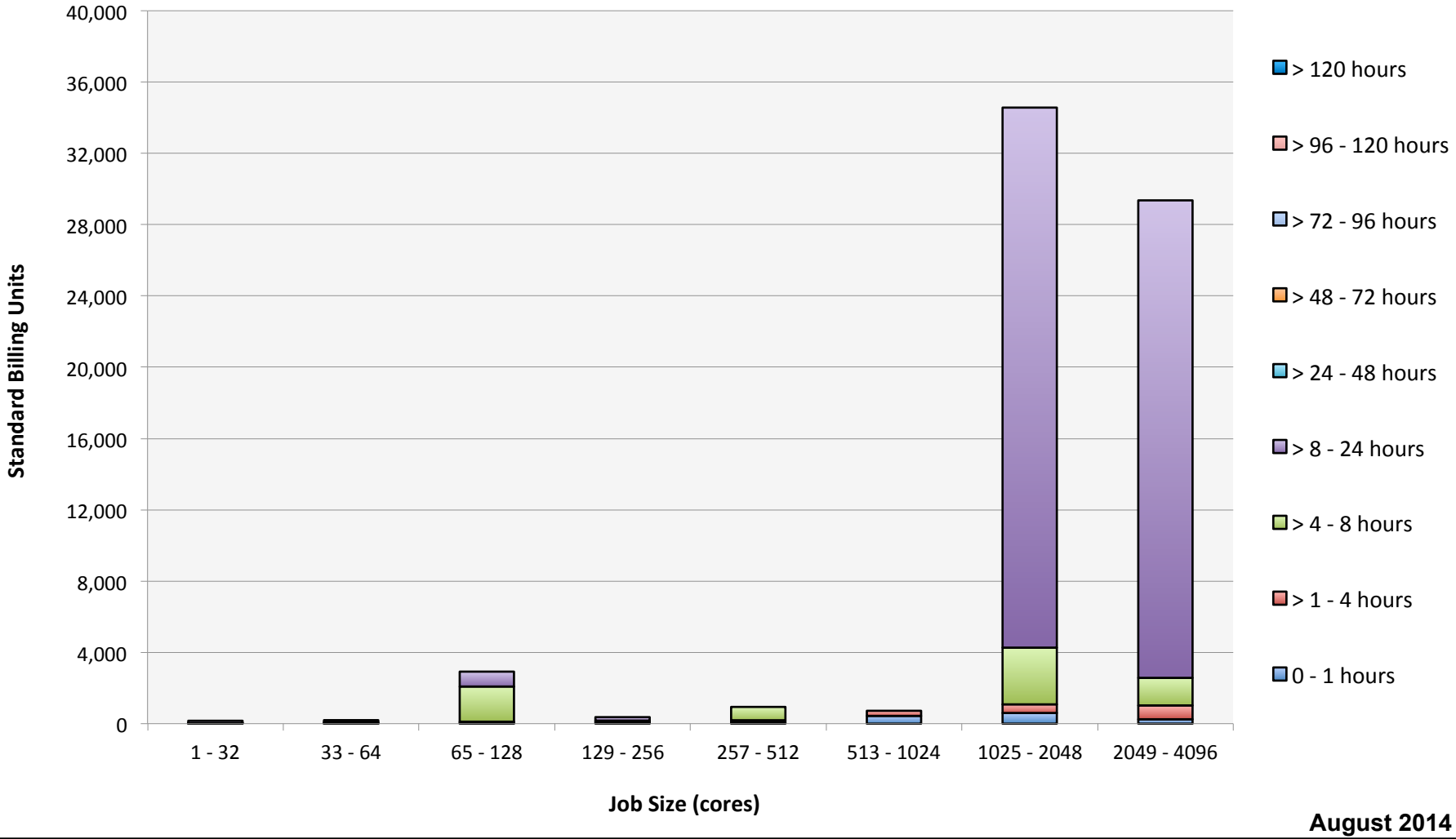
Merope:
Monthly Utilization by Job Length



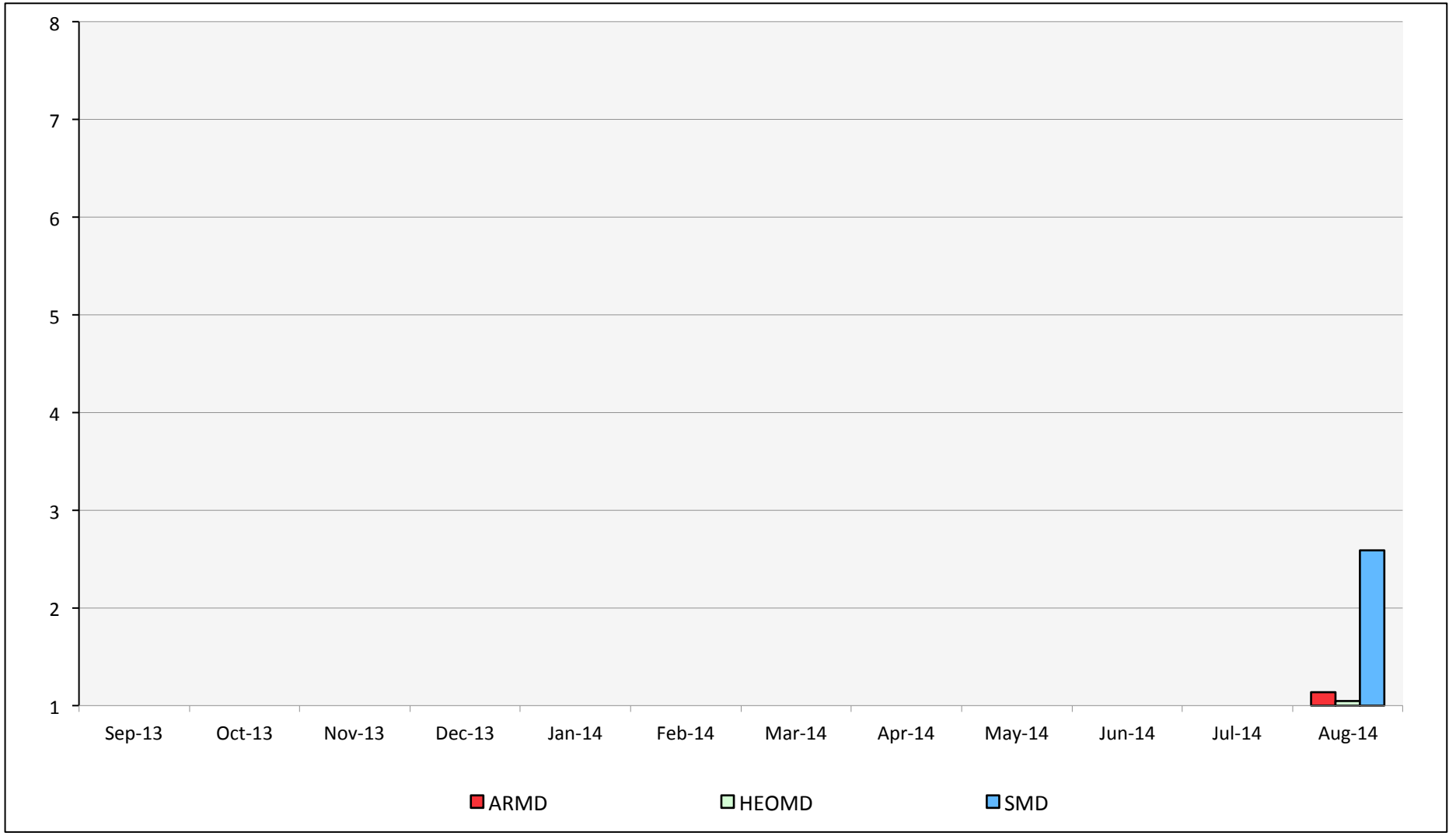
Merope:
Monthly Utilization by Size and Mission



Merope:
Monthly Utilization by Size and Length



Merope:
Average Expansion Factor



Maia:
SBUs Reported, Normalized to 30-Day Month