Project Status Report

High End Computing Capability
Strategic Capabilities Assets Program

May 10, 2015

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Merope Supercomputer Returned to Full Production

- HECC staff investigated and addressed several performance and stability issues adversely impacting the Merope cluster, operated from the auxiliary NASA Advanced Supercomputing (NAS) facility, one kilometer from the primary NAS facility.
- Merope uses a long-range InfiniBand (IB) extender to access the Lustre filesystem in the primary NAS facility. A new long-range Mellanox MetroX extender was deployed that resolved the Lustre issue.
- Changes were also made to the IB Subnet Manager relating to Quality of Service, to improve the performance and reliability of the IB fabric.
- HECC staff extensively tested the system to identify and correct performance issues from problematic compute nodes and subsystem components.
- The successful utilization of the MetroX long-range IB extender demonstrated the capability to connect HPC resources located in different locations—allowing more flexibility for future growth of HECC's computational capacity.

Mission Impact: Resolving performance and stability issues with the Merope supercomputer ensures that HECC can provide more compute cycles to scientists and engineers for NASA mission projects.

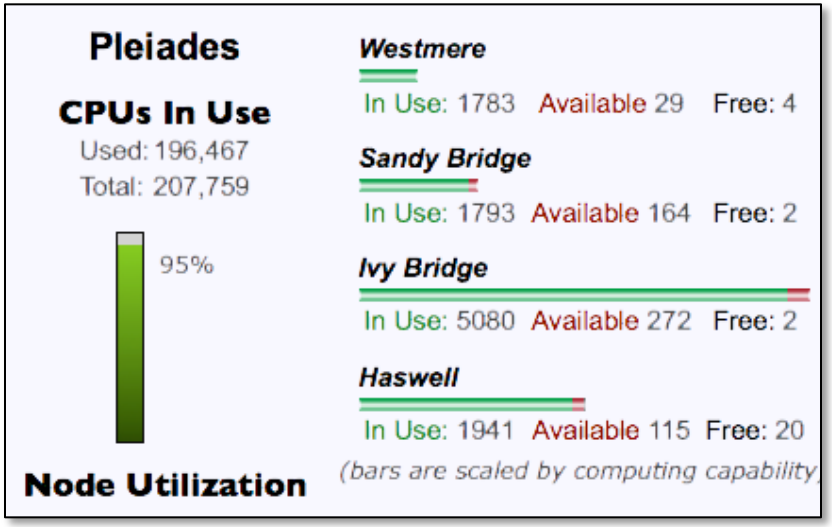
The Merope supercomputer consists of 704 Westmere and 448 Nehalem nodes that were retired from Pleiades due to power constraints. These nodes continue to provide computational cycles to HECC users in the secondary compute facility at NASA Ames.

POCs: Bob Ciotti, bob.ciotti@nasa.gov, (650) 604-4408, NASA Advanced Supercomputing Division; Davin Chan, davin.chan@nasa.gov, (650) 604-3613, NASA Advanced Supercomputing Division, Computer Science Corp

Additional PBSPro Scheduler Improves Pleiades' Responsiveness and Utilization

- HECC Supercomputing Systems staff, in collaboration with vendor staff from Altair, installed an additional PBS Professional scheduler, resulting in up to a 10x reduction in job-start wait time for users making improvements to their software on Pleiades.
- In the past, a single scheduler was responsible for all Pleiades jobs, resulting in wait times of about 10 minutes.
- A second scheduler is now in use that targets quick-starting user development jobs and other jobs intended for unique subsets of Pleiades nodes.
- The second scheduler consistently starts jobs within one minute if the job's requested resources are available, and reduced the workload of the first scheduler improving its turnaround time.

Mission Impact: Improvements in job scheduling performance assist systems engineers in keeping the HECC computational capability as fully utilized as possible, both for batch jobs and interactive use.



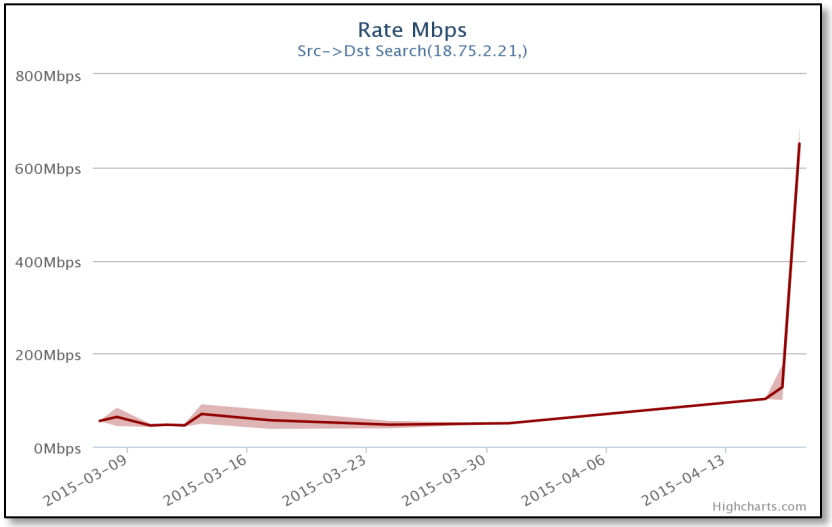
HECC staff maintain Pleiades utilization in the range of 90-plus percent, while meeting the resource requirements of users who need both quick turnaround for software development jobs and resources for large production jobs.

POC: Greg Matthews, gregory.matthews@nasa.gov, (650) 604-1321, NASA Advanced Supercomputing Division, Computer Sciences Corp.

Network Team Increases Data Transfer Rates to MIT By 18x

- HECC network engineers worked with system administrators at the Massachusetts Institute of Technology (MIT) to increase data transfer rates to MIT from 50 megabits per second (Mbps) to 900 Mbps peak, averaging around 700 Mbps.
- MIT staff provided a test server and HECC provided specific tuning parameters based on test results.
  - HECC installed the open-source HPN-SSH patch set to remove networking bottlenecks; and determined the best Transmission Control Protocol (TCP) congestion control algorithm to use between the sites.
  - Additionally, the network team identified CPU affinity bottlenecks and cryptographic overhead from ciphers that did not support multi-threading.
- HECC staff also tested a variety of data transfer applications to determine which offered the highest rates possible.
- The work prepares for transfers of large science datasets, including upcoming Kepler/TESS pixel data transfers (on the order of 1 terabyte every two weeks) between the NAS facility and MIT.

Mission Impact: By greatly increasing the network rates between the NASA Advanced Supercomputing (NAS) facility and the Massachusetts Institute of Technology, researchers working on NASA missions can quickly get results from datasets instead of waiting for days to transfer their data.



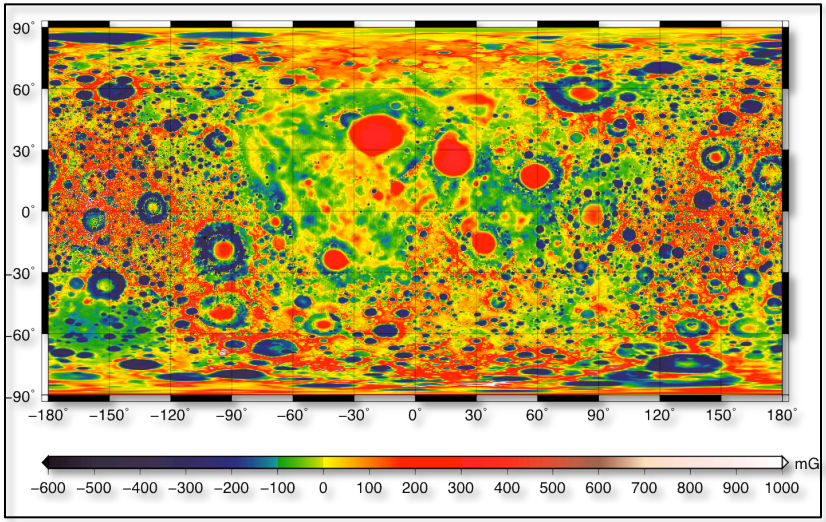
This graph shows the data transfer rate increase to the Massachusetts Institute of Technology system after specialized tuning.

POC: Nichole Boscia, nichole.k.boscia@nasa.gov, (650) 604-0891, NASA Advanced Supercomputing Division, Computer Sciences Corp.

HECC Staff Help Improve Reliability and Performance of GRAIL Project Runs

- HECC's Systems and Applications groups teamed up to help NASA's Gravity Recovery and Interior Laboratory (GRAIL) mission when runs of their "sfilter" code on Pleiades started failing earlier this year.
  - The Systems group adjusted InfiniBand settings and recommended that the GRAIL team make a change in communication libraries.
  - The Applications group recommended small changes in the I/O strategy used in sfilter, and also suggested changes in how processes are bound to cores on the nodes.
- The optimization changes resulted in a 10% improvement in the time required for GRAIL runs, which equates to about 60,000 Standard Billing Units (SBUs)* saved in March and April. The enhancements should save an additional 100,000 SBUs for runs remaining in the project year.
- More importantly, the GRAIL team reported that since jobs were again able to run to completion successfully, the result of HECC's help is a "100% improvement."

Mission Impact: HECC expertise in addressing application issues regularly results in performance boosts and much faster turnaround time for scientists and engineers across all mission directorates.



This map shows the gravity field of the moon as measured by NASA's Gravity Recovery and Interior Laboratory (GRAIL) mission. Units are in milligalileos (gal), where 1 gal is 1 centimeter per second squared. Red corresponds to mass excesses that create areas of higher local gravity, and blue corresponds to mass deficits that create areas of lower local gravity.

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

POC: Dan Kokron, daniel.kokron@nasa.gov, NASA Advanced Supercomputing Division, Computer Sciences Corp.

Construction Progresses on New NAS Cooling Tower

•HECC facilities engineers are working with Ames engineering staff to design and build a cooling tower for the primary NAS facility (building N258), which will replace the cooling tower located on land that Google leased from NASA Ames.

•The design was completed and approved in June 2014 and construction began in November 2014. The following milestones are complete:

- Electrical conduits located during excavation were encased in concrete for their protection.
- Sub-grade pea-gravel was grout-injected to provide a stable base to support the cooling tower structure.
- Trenching and measuring for the 20"-diameter water pipes is complete, and pipes are being fabricated to actual site dimensions.
- Concrete mat slab was poured and cured over compacted backfill, with 180 yards of concrete.
- First-level interior and exterior walls are poured and cured.
- Reinforcing steel for tower columns to support the second level are installed.

•The existing cooling tower is almost 30 years old. The new cooling tower will provide additional redundancy (for example, to compartmentalize the cooling tower basin), more efficient cooling, and all-new components (pumps, piping, and more).

Mission Impact: The new cooling tower replaces aging infrastructure, removes the old cooling tower from Google-leased property, and provides added redundancy and cooling efficiency to the NASA Advanced Supercomputing facility.

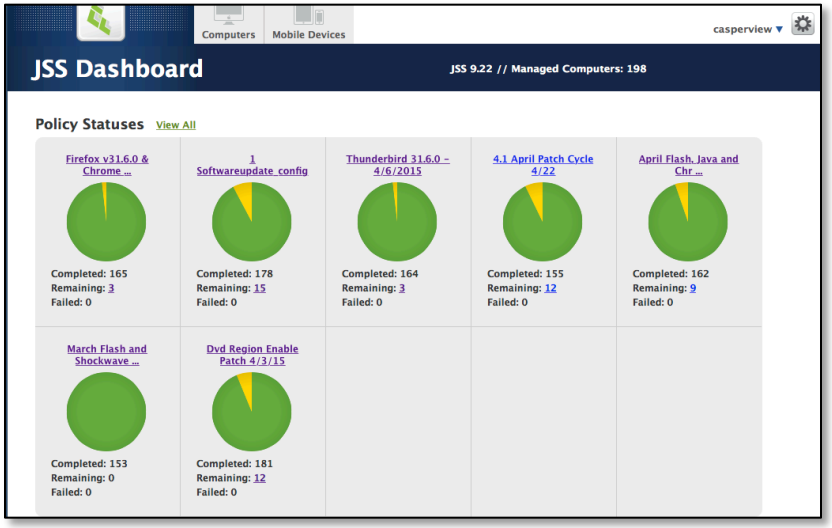
A recent photograph of the new HECC cooling tower construction. So far, the site is prepped, the mat slab (foundation) poured, and most of the first-level interior and exterior walls poured. The existing cooling tower can be seen directly behind the new tower.

POC: Chris Buchanan, chris.buchanan@nasa.gov, (650) 604-4308, NASA Advanced Supercomputing Division, Computer Sciences Corp.

Support Teams Improve Patch Management Tools and Processes

- Over the past several years, the frequency of patches to HECC systems has increased dramatically. HECC system administrators are implementing ways to decrease the time to apply system patches and manage an increasing number of patch requirements.
- For example, the Engineering Servers and Services (ESS) team deployed 55 Red Hat Linux and Mac OS X patch sets in FY13; 84 in FY14; and expects to deploy about 135 in FY15. This is over a 50% increase in the number of patch sets each year.
- In the past six months, the ESS team spent over 600 hours developing and deploying Red Hat Linux and Mac OS X patches, plus additional weeks of time tracking laptops that were not online during the scheduled patching time.
- Red Hat Linux patching is managed via a in-house script that queries the patch server for outstanding patches, updates drivers, and then runs “cfengine” for cleanup. The graphical user interface on the local patch server can be queried to check systems for missing patches.
- In addition, the HECC Security team is developing a patch reporting system, called the Host Assessment and Reporting Portal (HARP), which will provide system administrators with criticality levels, hosts affected, and specific applications that require patching. HARP will map patches to specific vulnerabilities associated with each patch.
- These support teams will continue improving the tools and processes associated with patch management in order to stay ahead of ever-increasing threats to HECC computational resources. For example, HARP is scheduled to go into production in June 2015

Mission Impact: By speeding up the process of applying patches to systems, HECC system administrators increase their ability to manage patches and reduce the risk of successful attacks on critical HECC computational resources.



This chart shows the output of a patch-management tool called Casper, which provides system administrators with information related to the patch status of OS X systems. This is one example of the tools deployed and/or developed by HECC system administrators to improve patch management.

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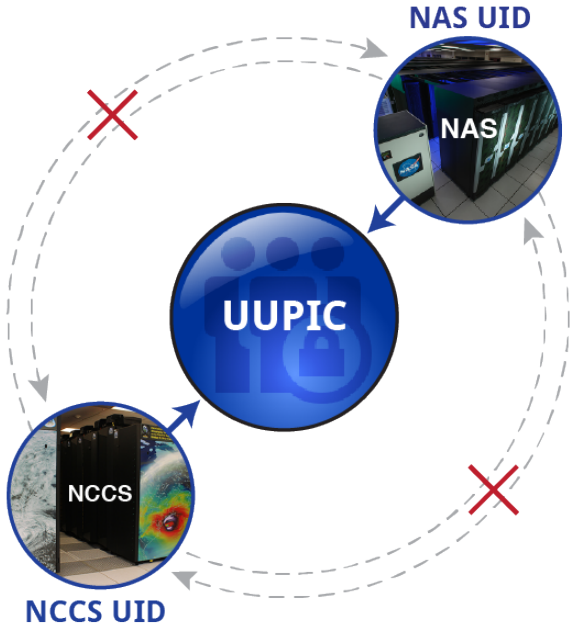
HECC Using Agency Universal Uniform Personal Identification Code as User ID

- The NAS facility and NASA Center for Climate Simulation (NCCS) streamlined the account creation process by now using the NASA Universal Uniform Personal Identification Code (UUPIC) as the user identification number (UID)—not username or login account (which are the users' AUIDs)—for all new users.
- A decade ago, when UUPICs were not used because some older computer systems could not handle the large values represented by 9-digit UIDs, NAS and NCCS agreed to give users the same UID at each site.
- In order to have the same UID at each site, before an account was created, one site had to contact the other to make sure the UID was not in use—causing delays in the account creation process.
- Having the same UID at each location makes it easier to move a user's jobs if needed for disaster recovery.
- Use of the UUPIC allows the UID to be determined simply by checking the user's identity in agency databases.

Mission Impact: Standardizing on the NASA Universal Uniform Personal Identification Code (UUPIC) reduces the amount of work that NAS and NCCS do on a daily basis in order to sync up user IDs across the two facilities, thereby making it faster for users to gain access to the systems.



Instead of using NAS user IDs and NCCS user IDs, both facilities now use the NASA Universal Uniform Personal Identification Code.

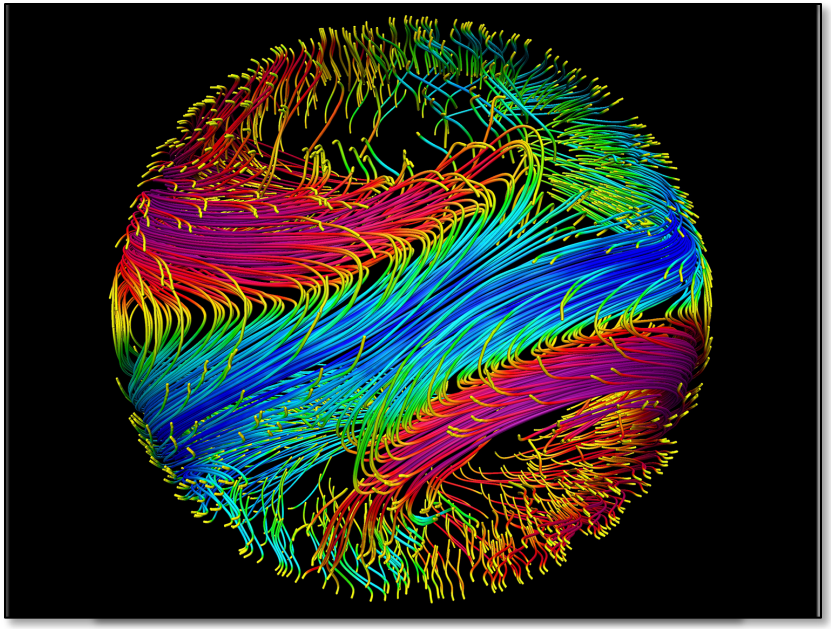
POC: Catherine Schulbach, catherine.h.schulbach@nasa.gov, (650) 604-3180, NASA Advanced Supercomputing Division

Simulations Provide Clues About the Interior Dynamics of Stars and Giant Exoplanets *

- Two groundbreaking simulation studies, run on the Pleiades supercomputer, revealed new information about the interior dynamics of stars and giant planets. These studies include:
  - The first self-consistent magnetohydrodynamic (MHD) simulations of a Jupiter-sized exoplanet close to its host star (known as a "hot Jupiter") that include both variable magnetic diffusivity and Ohmic heating.
  - The first 2D and 3D self-consistent MHD simulations of convectively driven internal gravity waves (IGWs) in a massive star.
- The simulation results showed that:
  - Magnetic effects may influence winds on hot Jupiters, and these effects might be observable through temperature maps. Also, unlike previously thought, Ohmic heating may not explain inflated radii observed on these exoplanets.
  - IGWs can alter a star's surface rotation and may explain some remaining mysteries, including observed chemical anomalies and differences between the orbits of planets around hot massive stars and those around cool ones.
- Each calculation required several hundred thousand to one million processor hours on Pleiades, resulting in about 60 terabytes of data.
- Analyses of these simulations can help astronomers interpret their observations and make predictions that will help guide future research.

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

Mission Impact: Simulations run on Pleiades help astronomers understand the massive influx of data from Earth- and space-based observatories, informing future observation decisions and helping researchers make the best use of NASA resources.



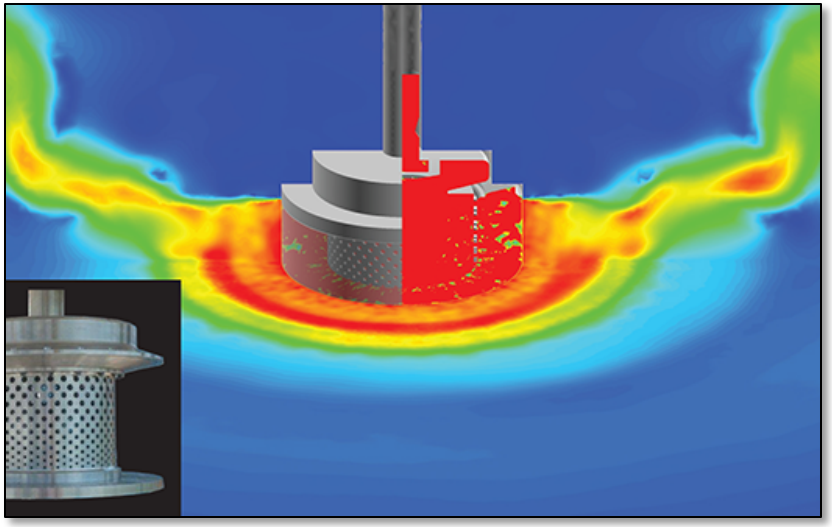
Magnetic field lines in a simulation of a "hot Jupiter" exoplanet. Magenta indicates toroidal magnetic fields with positive polarity; blue indicates fields with negative polarity.

POCs: Tami Rogers, tamara.rogers@ncl.ac.uk, +44 19 1208 7294, Newcastle University; Jess Vriesema,vriesema@lpl.arizona.edu, (520) 626-9846, University of Arizona

CFD Simulations Enable Efficient Optimization for Designing Complex Rocket Components *

- State-of-the-art computational fluid dynamics (CFD) simulations, run on Pleiades, enable complex hardware designs for launch vehicle rockets to be efficiently optimized before they are completed.
- Using the Loci-STREAM CFD code, researchers at Marshall Space Flight Center performed CFD analyses to optimize the design of a low-profile ullage gas diffuser (LPD), from an initial concept to a prototype. The Space Launch System baseline diffuser was also modeled. The researchers:
  - Generated detailed 3D models of about 20 diffuser designs and performed CFD simulations of each design in less than two months.
  - Conducted analyses of the final diffuser concept to provide pre-test performance predictions before the hardware was fabricated.
  - Provided pre-test performance predictions for flow tests of a large, traditionally designed (baseline) gas diffuser.
  - Generated a large-scale, ~700-million-cell mesh of the diffuser and performed time-accurate, 3D CFD simulations at two different flow conditions, in three months.
  - Designed, built, and successfully tested a prototype system.
- Each of the LPD concept simulations required a computational mesh with around 50 million cells and around 75,000 processor-hours to complete, while the CFD simulation of the traditionally designed (SLS) diffuser required a 700-million-cell mesh and 2.8 million processor-hours on Pleiades.

Mission Impact: Computational fluid dynamics design support for NASA's investment in rocket hardware would not be possible without access to large high-performance computing resources such as the Pleiades supercomputer.



Simulated velocity magnitude contour and hardware of a prototype low-profile gas diffuser.

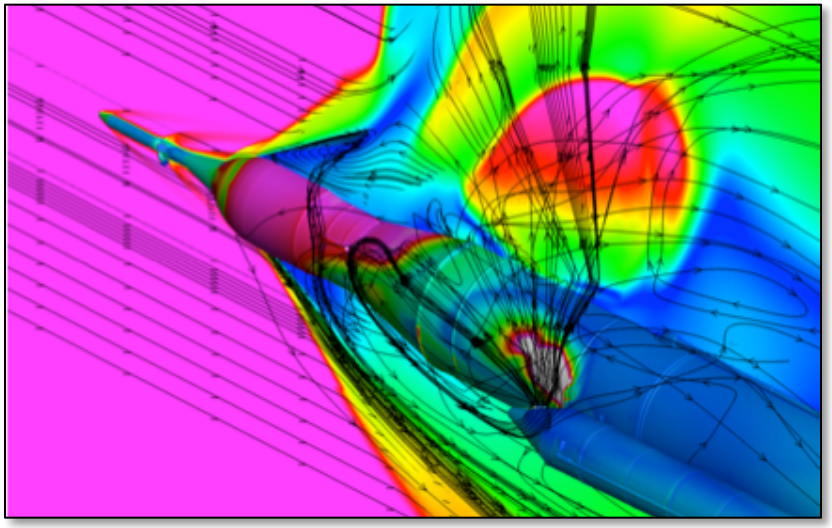
POC: Narayanan Ramachandran, narayanan.r.ramachandran@nasa.gov, (256) 544-8308, NASA Marshall Space Flight Center

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

CFD Simulations Support Assessment of Booster Separation Safety for SLS *

- NAS Division computational fluid dynamics (CFD) experts completed extensive simulations of early-phase booster separation for the Space Launch System (SLS) Design Analysis Cycle 3 (DAC3) Booster Separation Database. The research team:
  - Simulated nearly 11,800 cases covering the first 0.8 seconds/10 axial feet of separation.
  - Used a combination of the efficient Cart3D CFD code and the high-fidelity, viscous OVERFLOW CFD code.
  - Simulated wind tunnel test conditions with and without booster separation motor (BSM) plumes to validate CFD results and assess uncertainty levels.
  - Simulated full-scale flight condition cases with plumes from the BSMs, boosters, and core stage engines.
  - Delivered aerodynamic force and moment data, quality checks, and flow-field plots for each case.
- Using ~4.5 million core hours on Pleiades, these early-phase separation analyses were able to meet a prioritized deadline from the SLS chief engineer.
- Initial results indicate that the current DAC3 dataset has much lower uncertainty than the previous DAC2 dataset, which will enable more accurate assessment of potential booster recontact risks.

Mission Impact: HECC resources enabled the delivery of critical aerodynamic data needed to assess the risk of recontact during booster separation and confirm the safety and effectiveness of the booster separation system design for the SLS.



OVERFLOW simulation of SLS booster separation, showing flow-field particle traces, flow-field Mach contours, and surface pressure contours on the vehicle.

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

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

HECC Facility Hosts Several Visitors and Tours in April 2015

- HECC hosted 10 tour groups in April; 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:
  - Dave Radzanowski, NASA NASA Chief Financial Officer.
  - Attendees of the Aerospace Flutter and Dynamics Council meeting, hosted by the Ames Research Center (ARC) Exploration Technology Directorate.
  - Members of the 63rd Army Reserve Judge Advocate General's Corps, as part of their ARC tour;
  - A group of NASA researchers who attended the Big Data Big Think II Working Group, hosted by NAS Division Chief Piyush Mehrotra and NASA Chief Technology Officer Deborah Diaz.
  - A group of Google staff including, Director of Engineering Hartmut Neven, visited the HECC facility and Quantum Artificial Intelligence Laboratory to view the upgraded quantum system.
  - His Excellency Mr. Sebastian Kurz, Federal Minister of Foreign Affairs of the Austrian Foreign Ministry. along with Ambassador Hans Peter Manz, Consul General Ulrike Ritzinger, and 35 additional members of the delegation, received tours and presentations from NASA staff at the NAS facility.

Chris Henze, data analysis and visualization expert in the NASA Advanced Supercomputing (NAS) Division, discusses the science behind visualizations displayed on the hyperwall system to a group of NASA researchers visiting Ames for the Big Data Big Think II meeting.

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

Papers

- "**Generation of Magnetic Holes in Fully Kinetic Simulations of Collisionless Turbulence**," V. Roytershteyn, H. Karimabadi, A. Roberts, Philosophical Transactions A, vol. 373, issue 2041, Early online publication April 6, 2015. * *http://rsta.royalsocietypublishing.org/content/373/2041/20140151.abstract*
- "**A One-Dimensional Model for Rayleigh-Taylor Instability in Supernova Remnants**," P. Duffell, arXiv:1504.02200 [astro-ph.HE], April 9, 2015. * *http://arxiv.org/abs/1504.02200*
- "**Sweating the Small Stuff: Simulating Dwarf Galaxies, Ultra-Faint Dwarf Galaxies, and Their Own Tiny Satellites**," C. Wheeler, et al., arXiv:1504.02466 [astro-ph.GA], April 9, 2015. * *http://arxiv.org/abs/1504.02466*
- "**Magnetic Flux Conservation in the Heliosheath Including Solar Cycle Variations of Magnetic Field Intensity**," A. Michael, M. Opher, E. Provornikova, J. Richardson, G. Toth, The Astrophysical Journal Letters, vol. 803, no. 1, April 10, 2015. * *http://iopscience.iop.org/2041-8205/803/1/L6*
- "**Orientation of X-Lines in Asymmetric Magnetic Reconnection—Mass Ratio Dependency**," Y.-H. Liu, et al., arXiv:1504.03300 [physics.space-ph], April 13, 2015. * *http://arxiv.org/abs/1504.03300*

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

Papers (cont.)

- "**Capture and Evolution of Planetesimals in Cicumjovian Disks**," G. D'Angelo, M. Podolak, arXiv:1504.04364 [astro-ph.EP], April 16, 2015. * *http://arxiv.org/abs/1504.04364*
- "**Dating the Moon-forming Impact Event with Asteroidal Meteorites**," W. Bottke, et al., Science Magazine, April 17, 2015. * *http://www.sciencemag.org/content/348/6232/321.short*
- "**Formation of Elongated Galaxies with Low Masses at High Redshift**," D. Ceverino, J. Primack, A. Dekel, arXiv:1504.04988 [astro-ph.GA], April 20, 2015. * *http://arxiv.org/abs/1504.04988*
- "**The Evidence for Slow Migration of Neptune from the Inclination Distribution of Kuiper Belt Objects**," D. Nesvorny, arXiv:1504.06021 [astro-ph.EP], April 23, 2015. * *http://arxiv.org/abs/1504.06021*

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

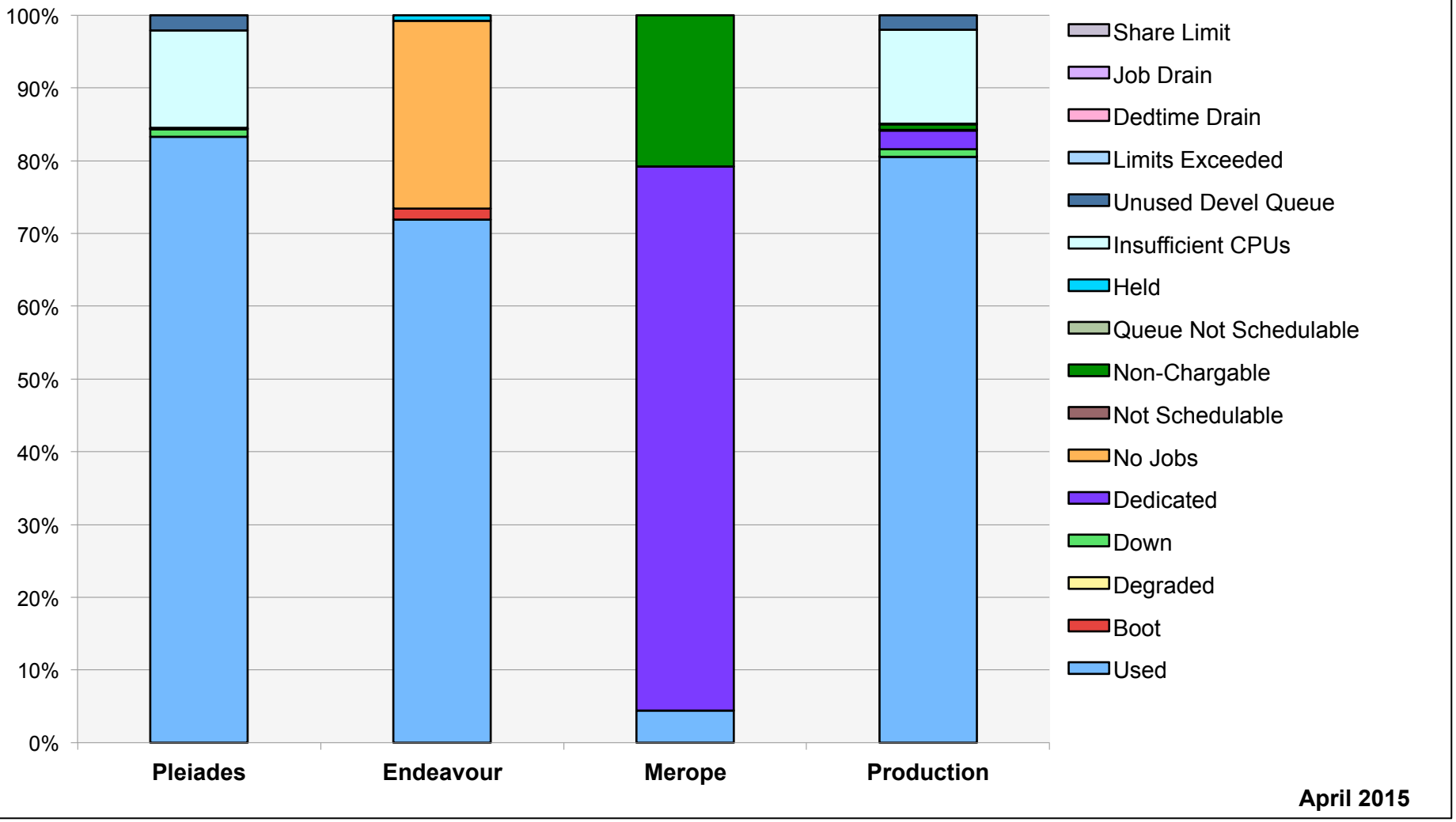
Presentations

- "**Fast Database Generation for Parachute Cluster Design Using Navier-Stokes Equations on Supercomputers**," G. Guruswamy, presented at the 23rd AIAA Aerodynamic Decelerator Systems Technology Conference, Daytona Beach, FL, March 30 – April 2, 2015. *http://arc.aiaa.org/doi/pdf/10.2514/6.2015-2170*
- **"Big Data @ NASA: Challenges and Opportunities."** P. Mehrotra, presented at the Deep Space Deep Ocean, Houston, TX April 6-7, 2015
- "**Sensitivity of Ground Damage Predictions to Meteroid Breakup Modeling Assumptions**," D. Mathias, presented at the 2015 IAA Planetary Defense Conference, Frascati, Italy, April 13-17, 2015.
- "**Dynamic Simulation Probabilistic Risk Assessment Model for an Enceladus Sample Return Mission**," C. Mattenberger, D. Mathias, K. Gee, presented at the 2015 International Topical Meeting on Probabilistic Safety Assessment and Analysis (PSA), Sun Valley, ID, April 26-30, 2015.

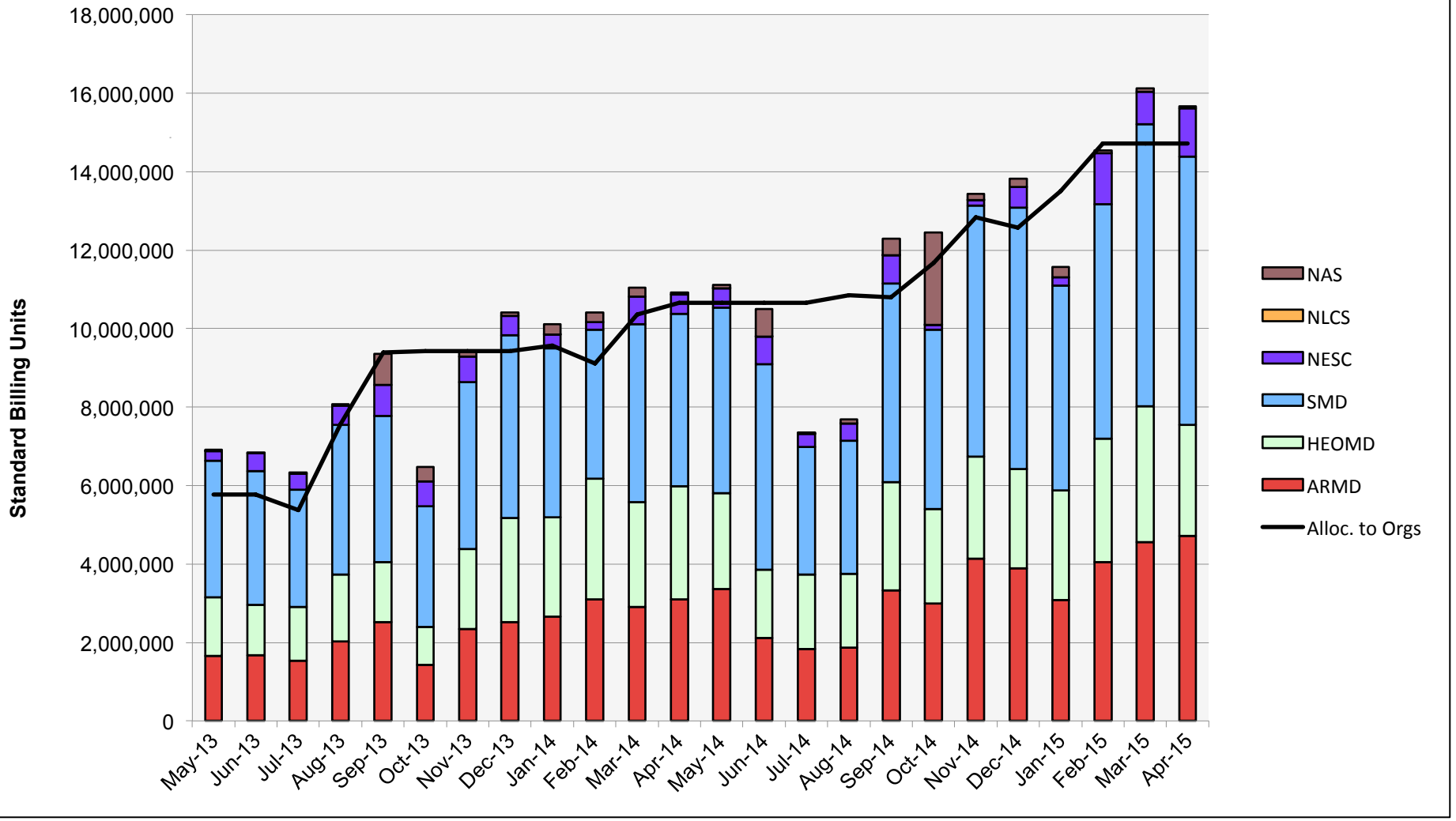
News and Events

- **3D Printing Reveals Never-Before-Detected Details of Superstar Eta Carinae**, *Cutting Edge: Goddard's Emerging Technologies (Spring 2015)*—NASA Goddard's Thomas Madura used 3D printing to create models of Eta Carinae based on simulations run on the Pleiades supercomputer, discovering never-before-revealed details about the star system. *http://gsfctechnology.gsfc.nasa.gov/3DPrinting.html*
- **NASA Ames Research Center to Support Advanced Computing Services**, *HPCwire*, April 6, 2015—NASA Ames Research Center announced plans to procure services to support the advanced computing services provided by the NASA Advanced Supercomputing (NAS) Division. *http://www.hpcwire.com/off-the-wire/nasa-ames-research-center-to-support-advanced-computing-services/*
- **Chinese Supercomputer 'Too Slow' to Compete in Race for Hypersonic Weapons, Scientist Warns**, *South China Morning Post*, April 24, 2015—A researcher at China's state laboratory of aerodynamics at Mianyang said that top priority hypersonic weapons research in China does not always get access to the country's top supercomputers, many of which were not created to meet specific needs of scientists and engineers. He added that the hypersonic project's supercomputer would have to increase its performance 10 times to match its U.S. counterpart, the Pleiades supercomputer. *http://www.scmp.com/tech/science-research/article/1773421/chinese-supercomputer-too-slow-compete-race-hypersonic-weapons*

HECC Utilization



HECC Utilization Normalized to 30-Day Month



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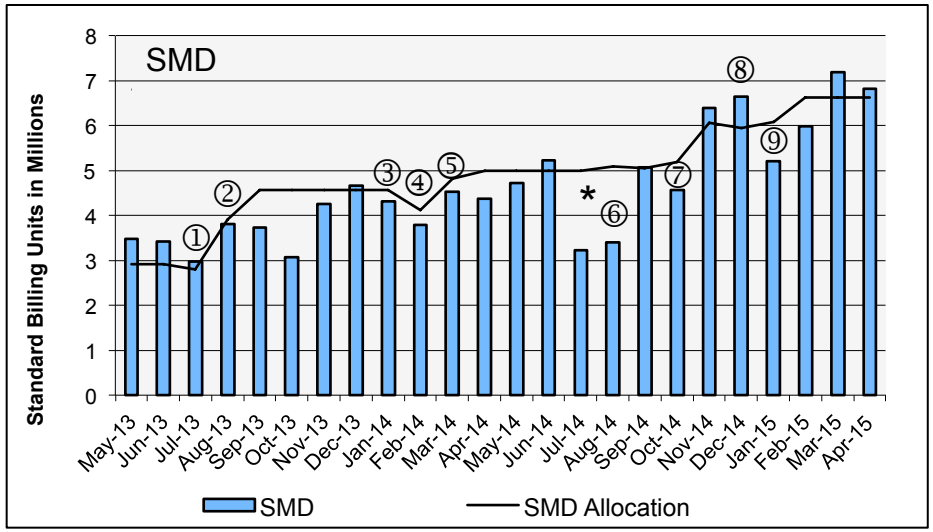
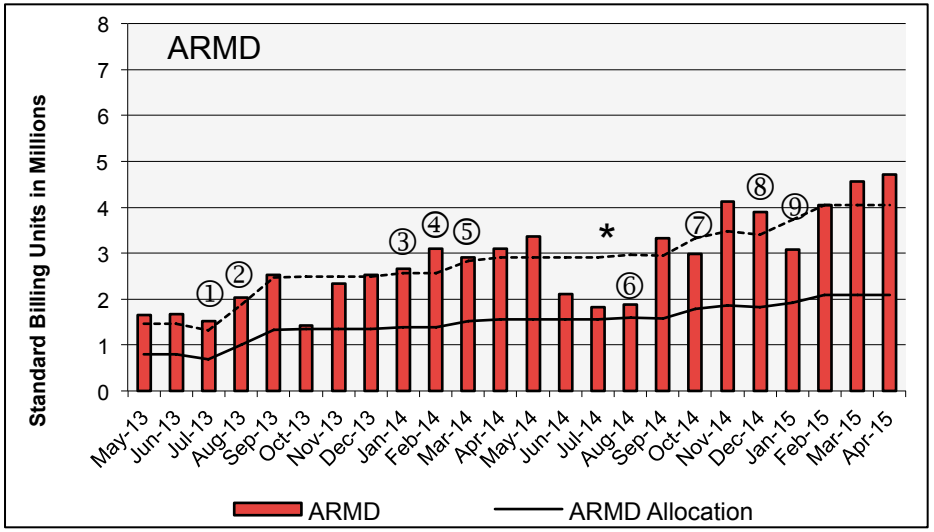
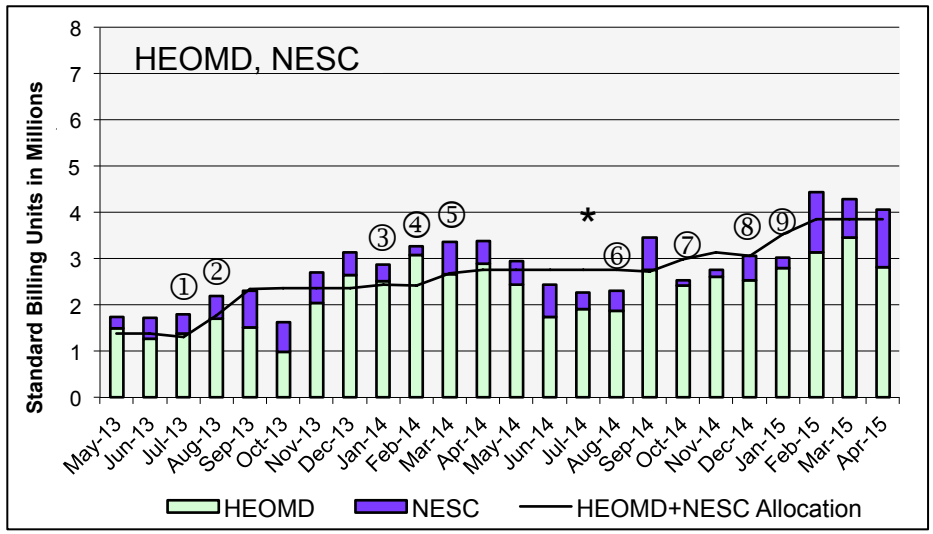






① 32 Harpertown Racks retired

② 32 Harpertown Racks retired; 46 Ivy Bridge Racks added

③ 6 Ivy Bridge Racks added; 20 Nehalem, 12 Westmere Racks Retired

④ 8 Ivy Bridge Racks added mid-Feb; 8 Ivy Bridge Racks added late Feb.

⑤ 4 Ivy Bridge Racks added mid-March

⑥ 6 Westmere Racks added to Merope, Merope Harpertown retired

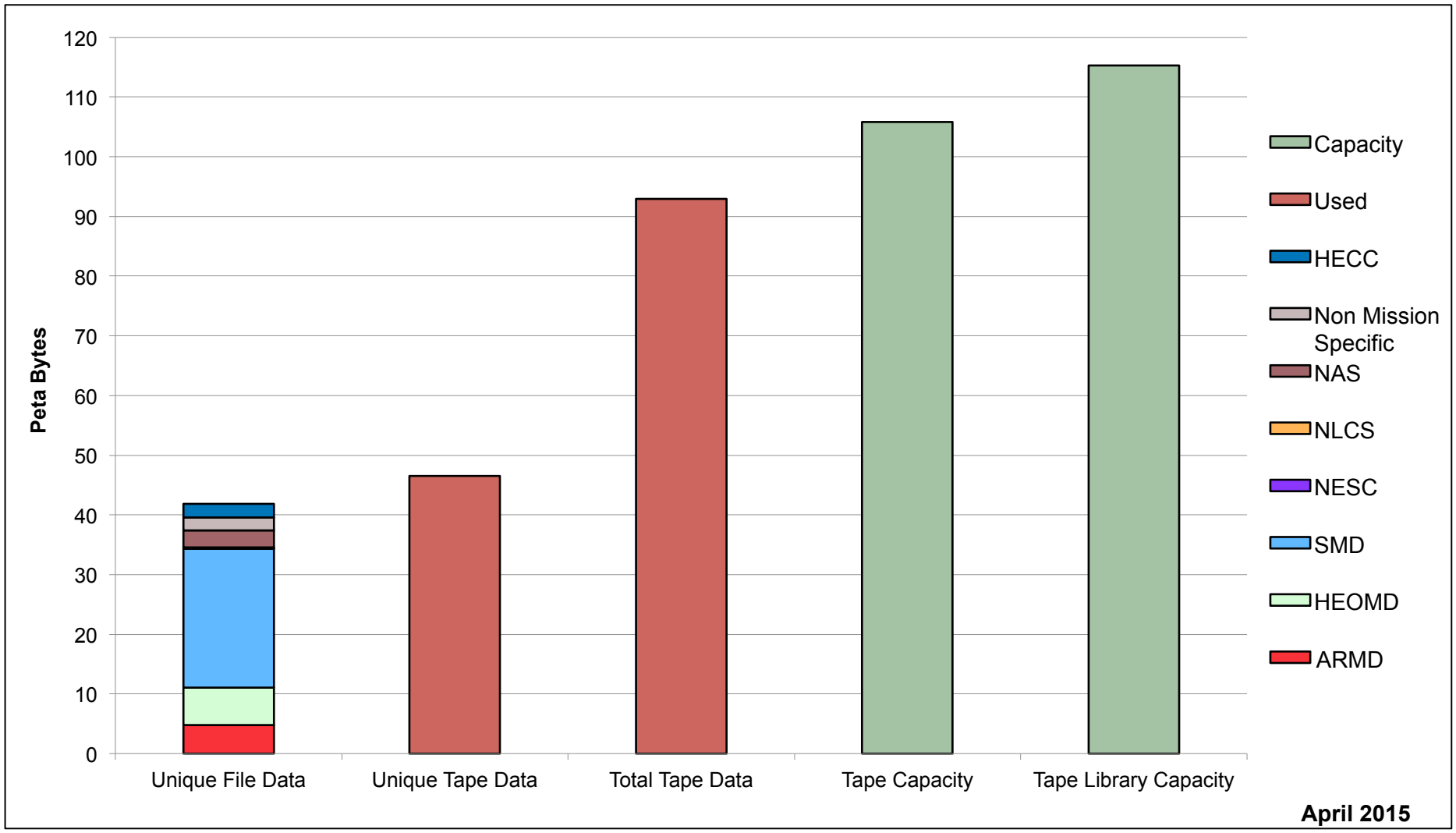
⑦ 16 Westmere Racks retired; 10 Nehalem Racks and 2 Westmere Racks added to Merope; 3 Ivy Bridge Racks added; 15 Haswell Racks added

⑧ 16 Westmere Racks retired

⑨ 14 Haswell racks added

* 1/2 of Pleiades was turned off in July and August due to cooling tower issues

Tape Archive Status



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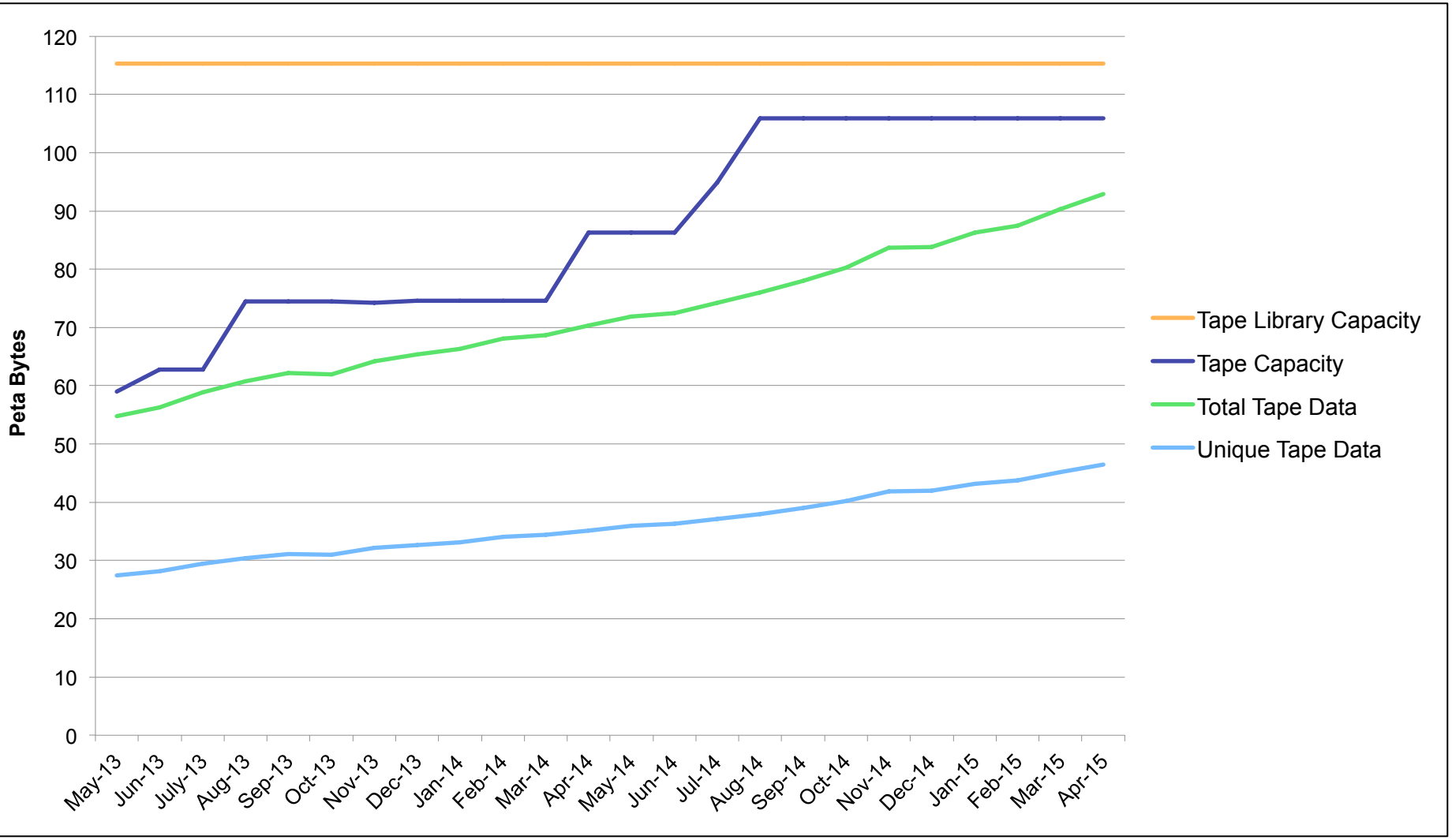
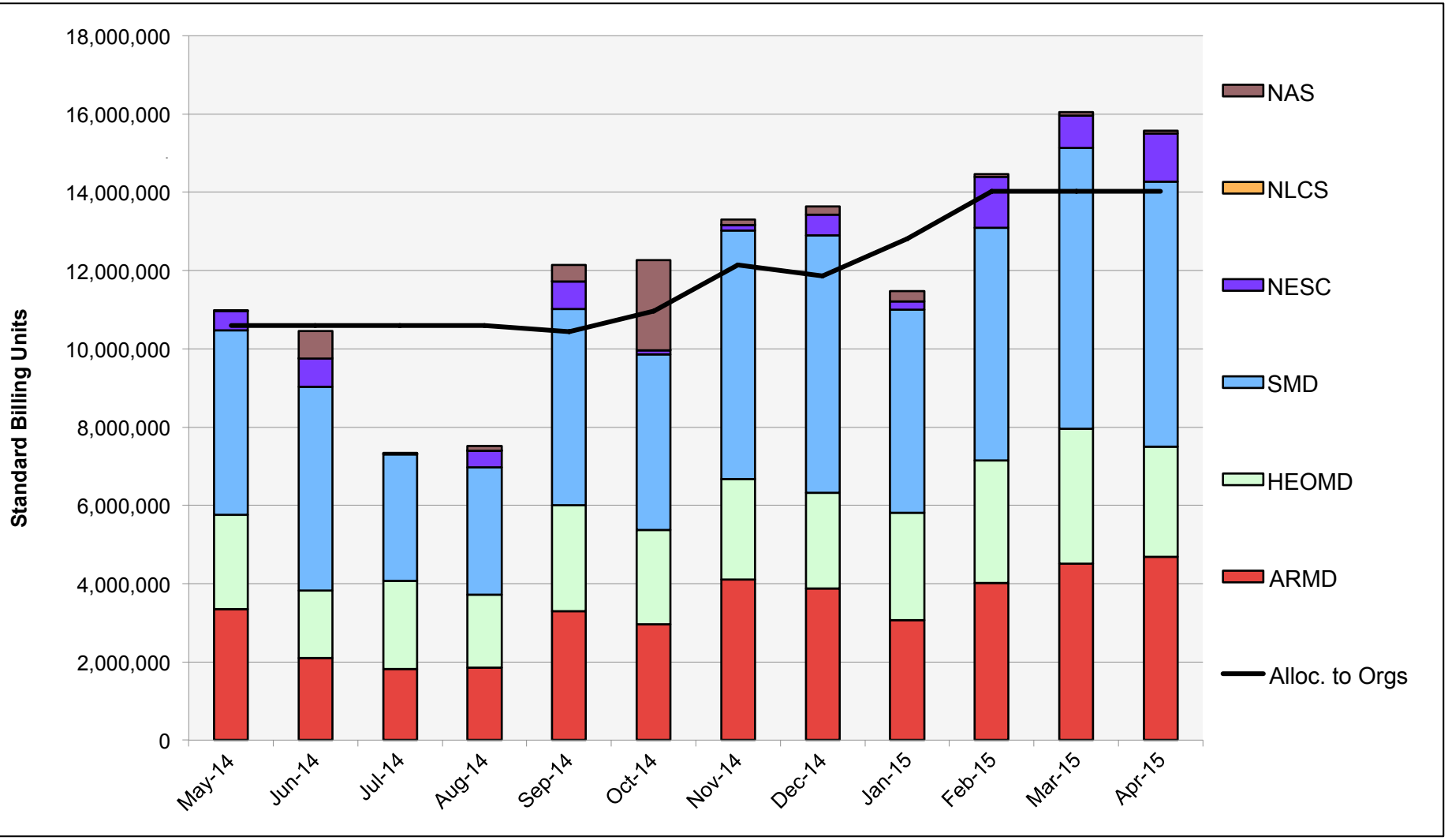
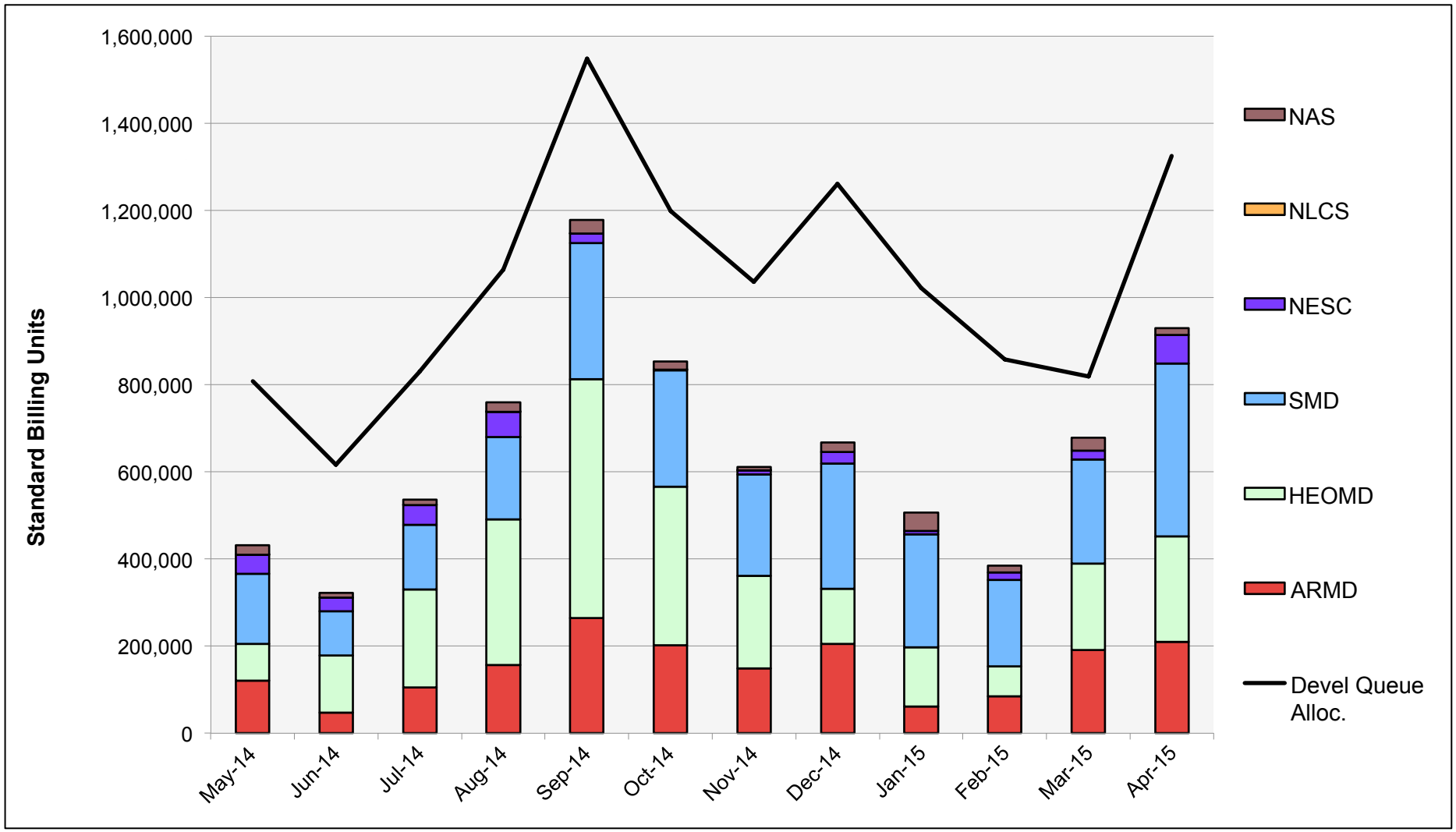


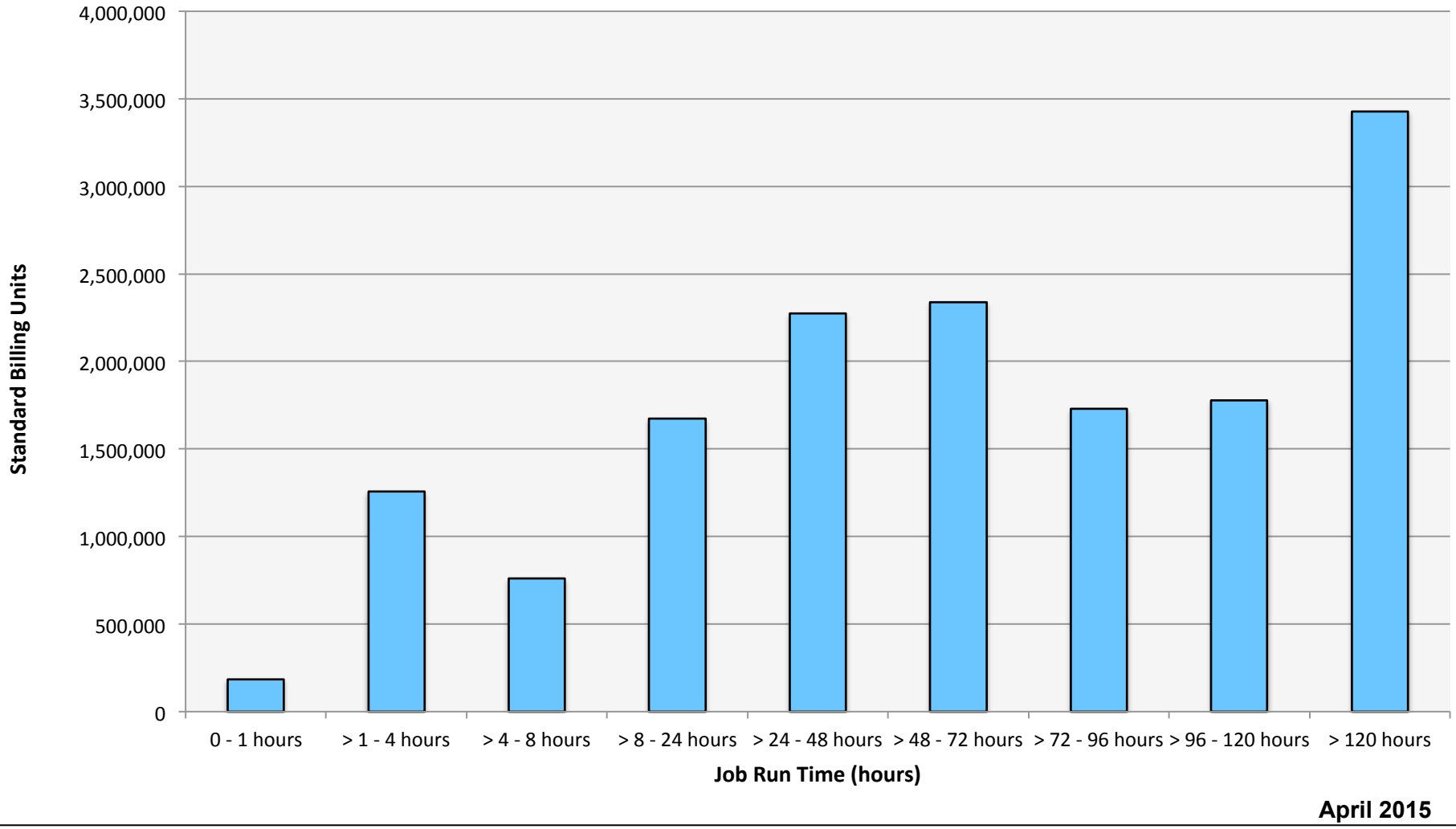
Pleiades:
SBUs Reported, Normalized to 30-Day Month



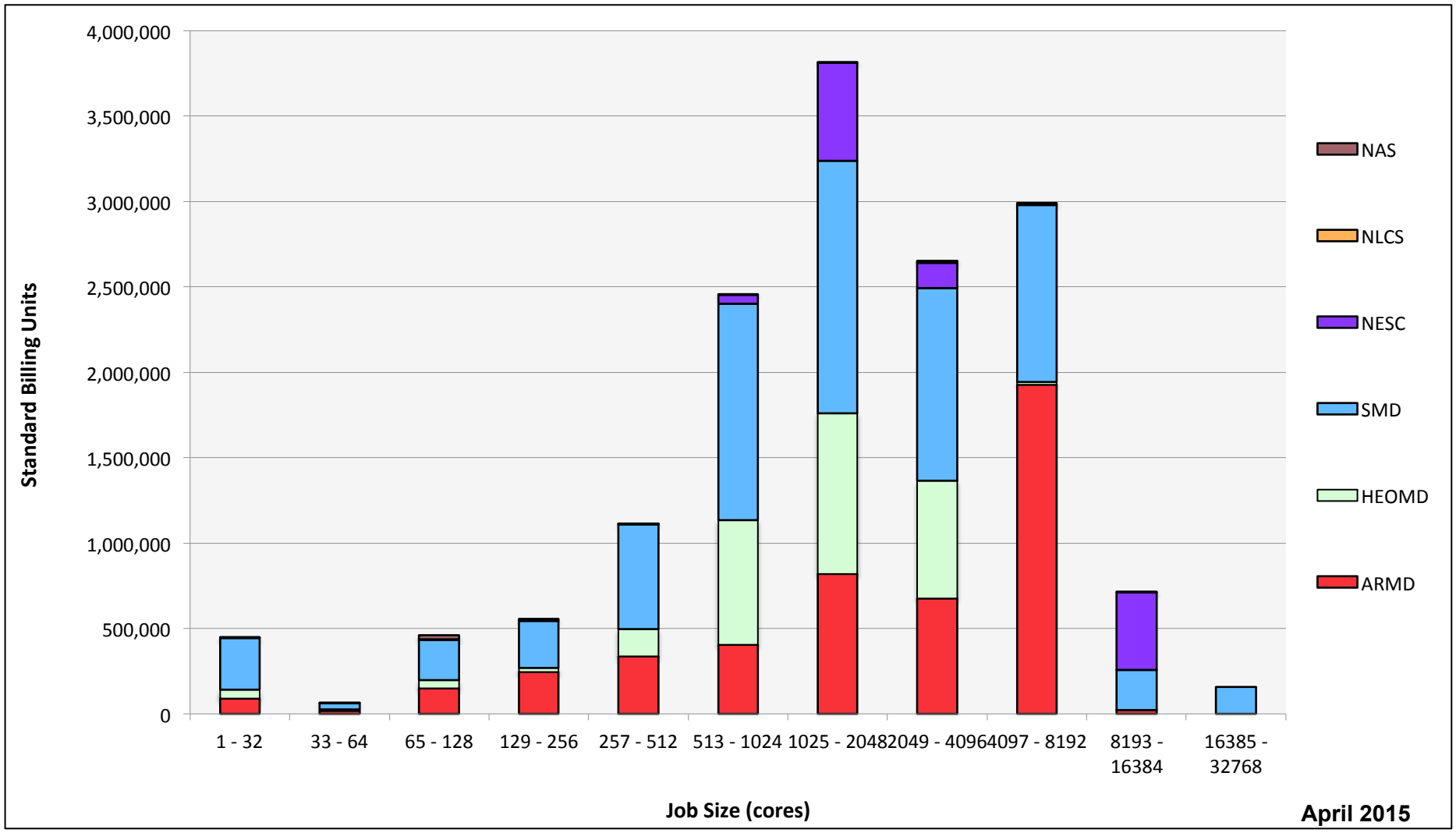
Pleiades:
Devel Queue Utilization



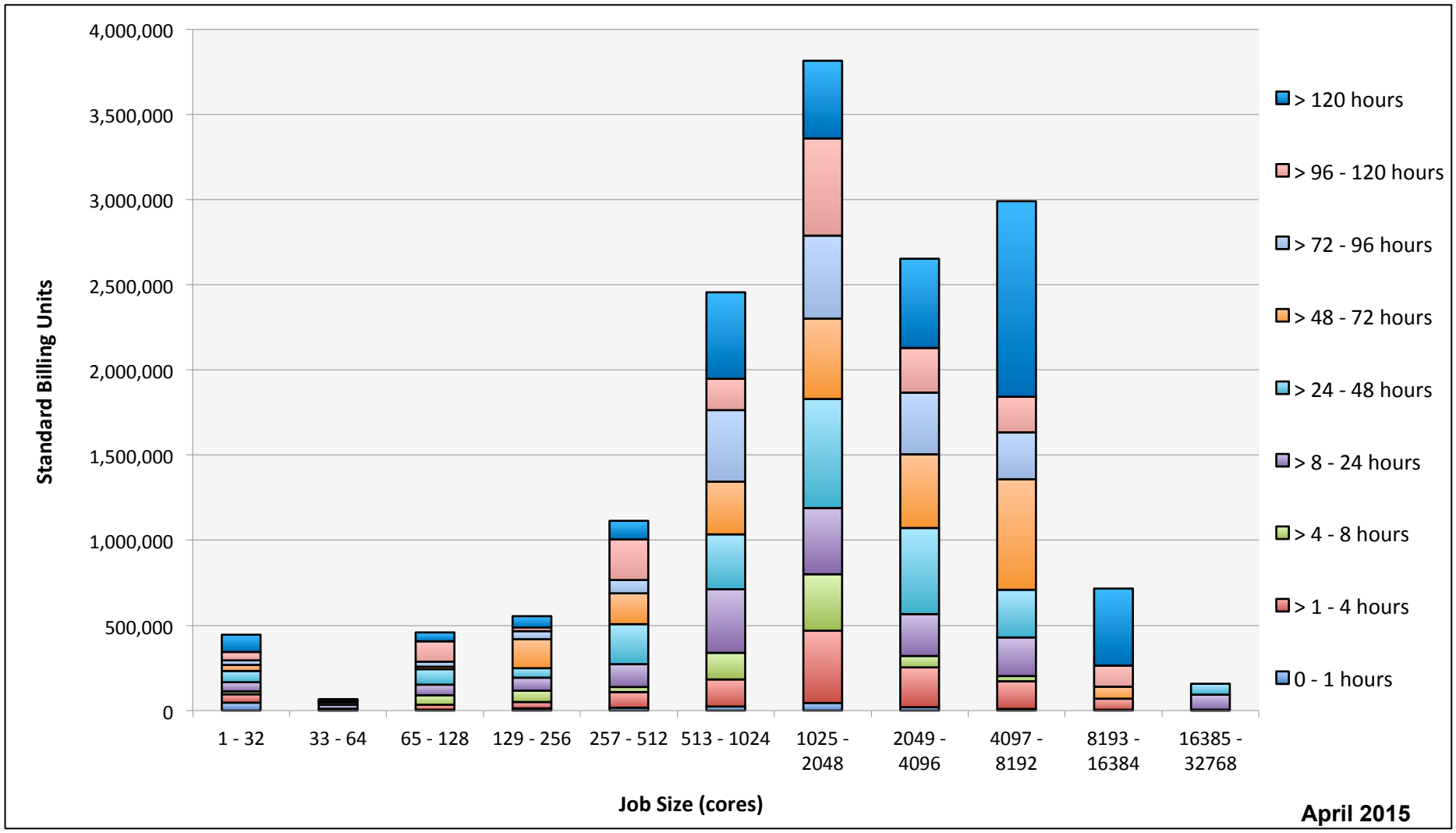
Pleiades:
Monthly Utilization by Job Length



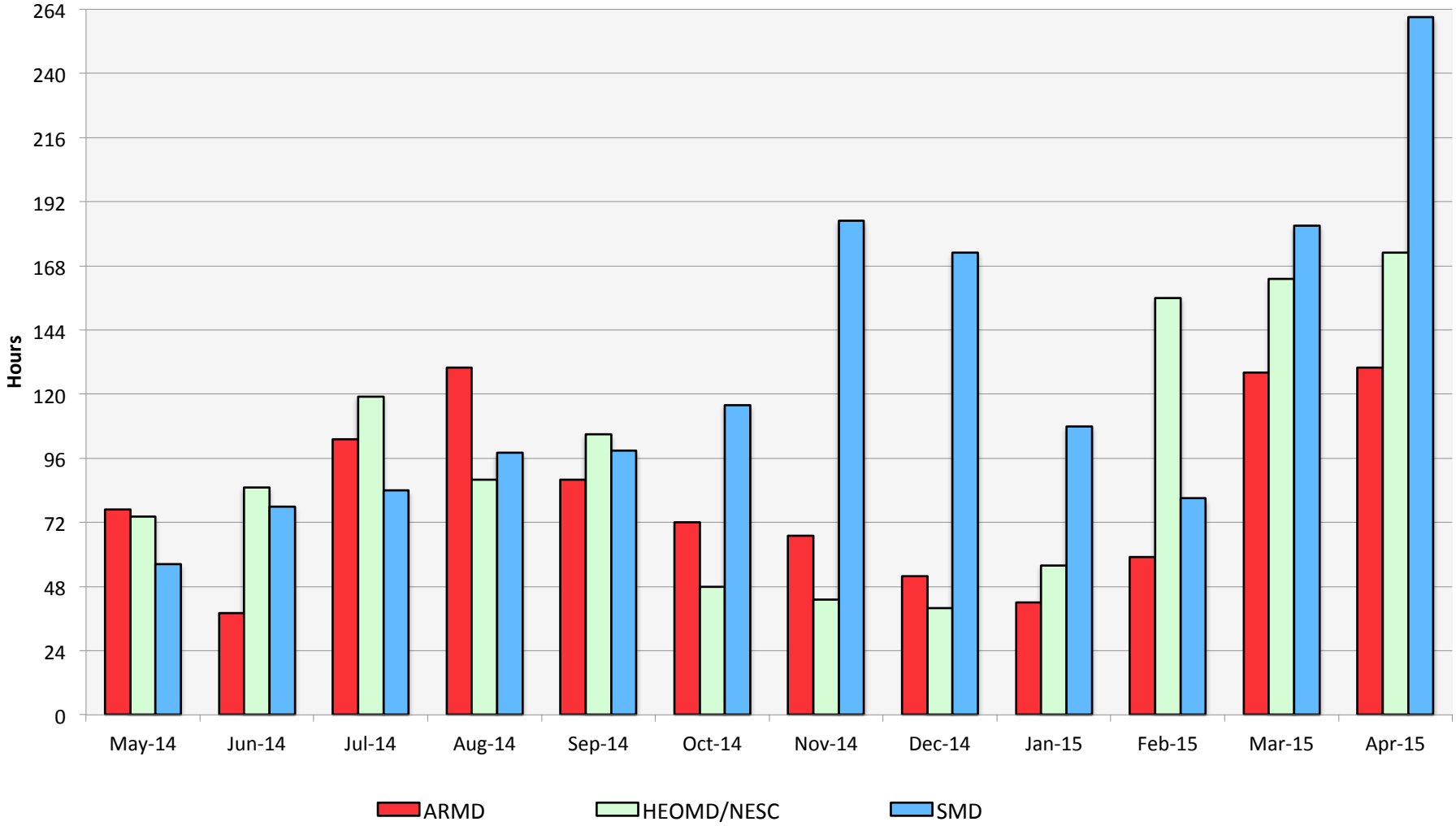
Pleiades:
Monthly Utilization by Size and Mission



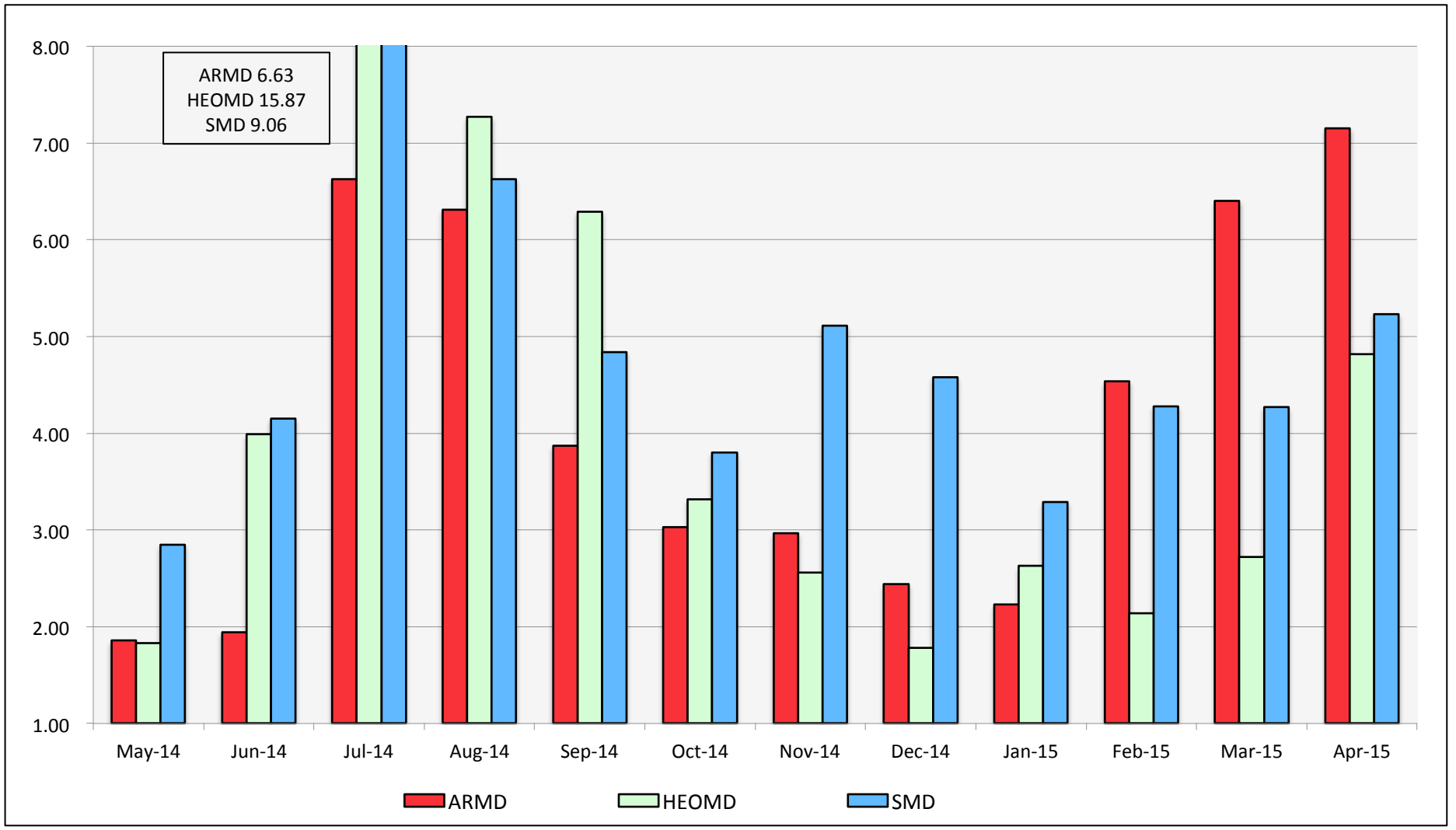
Pleiades:
Monthly Utilization by Size and Length



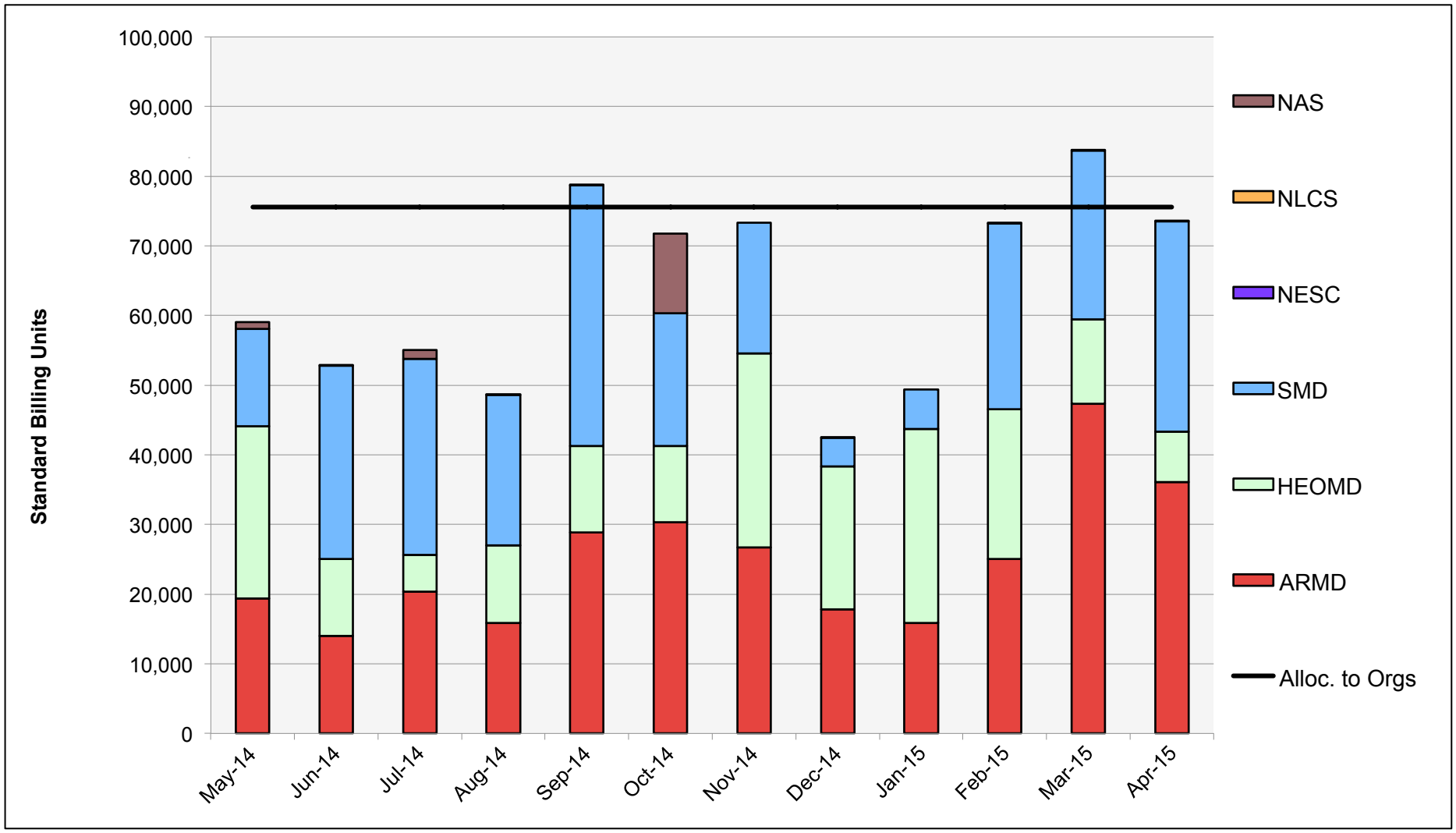
Pleiades:
Average Time to Clear All Jobs



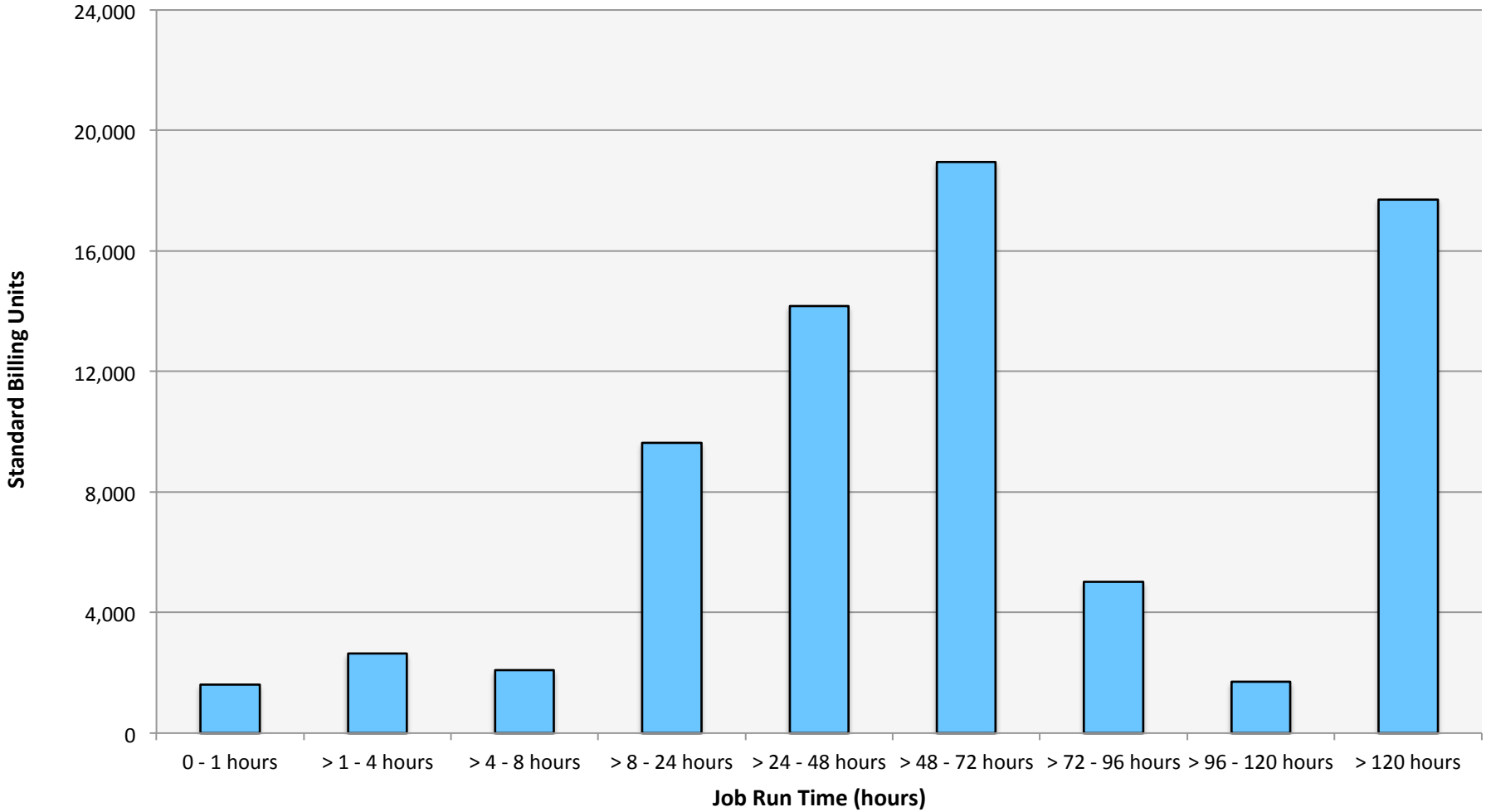
Pleiades:
Average Expansion Factor



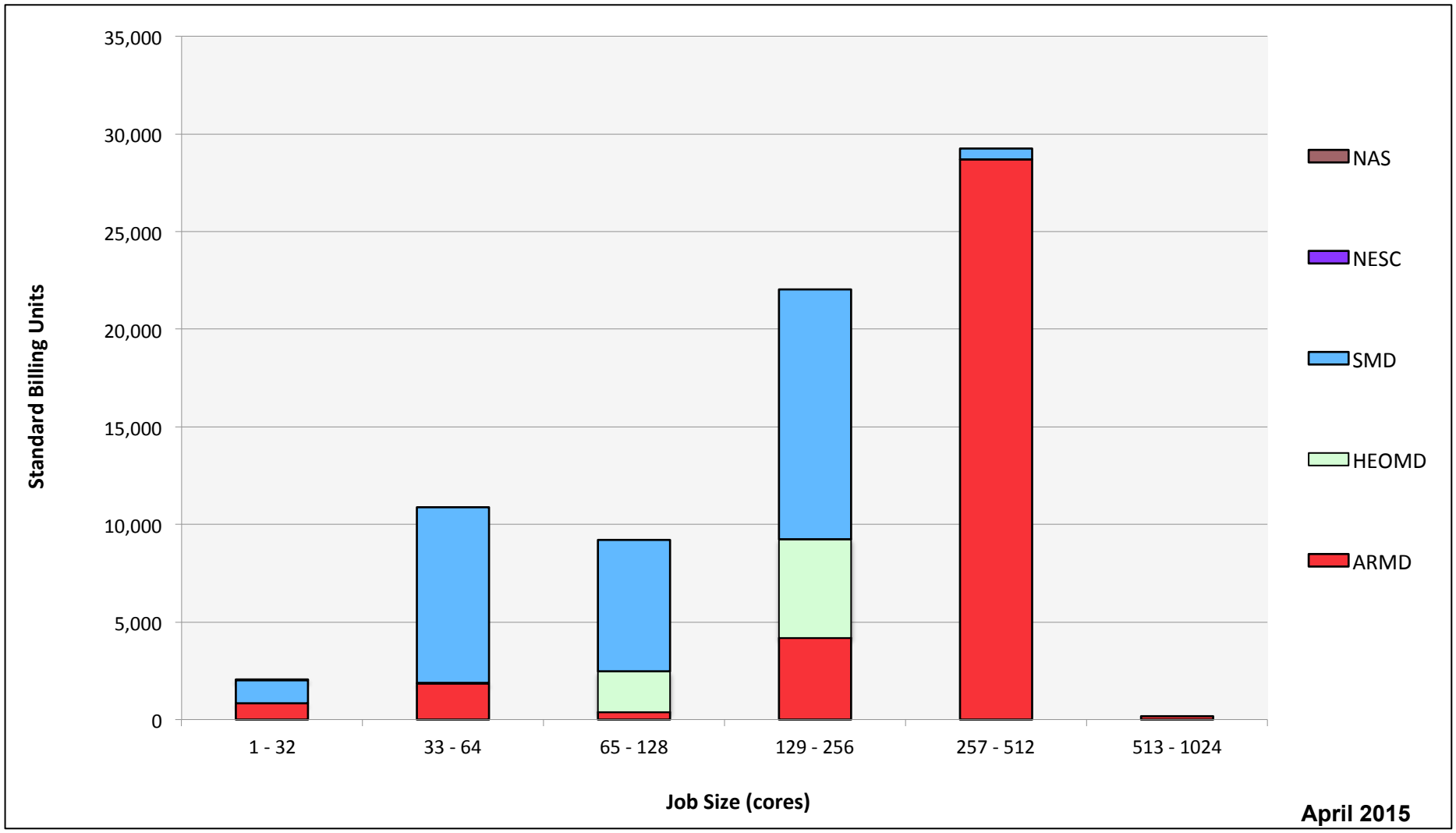
Endeavour:
SBUs Reported, Normalized to 30-Day Month



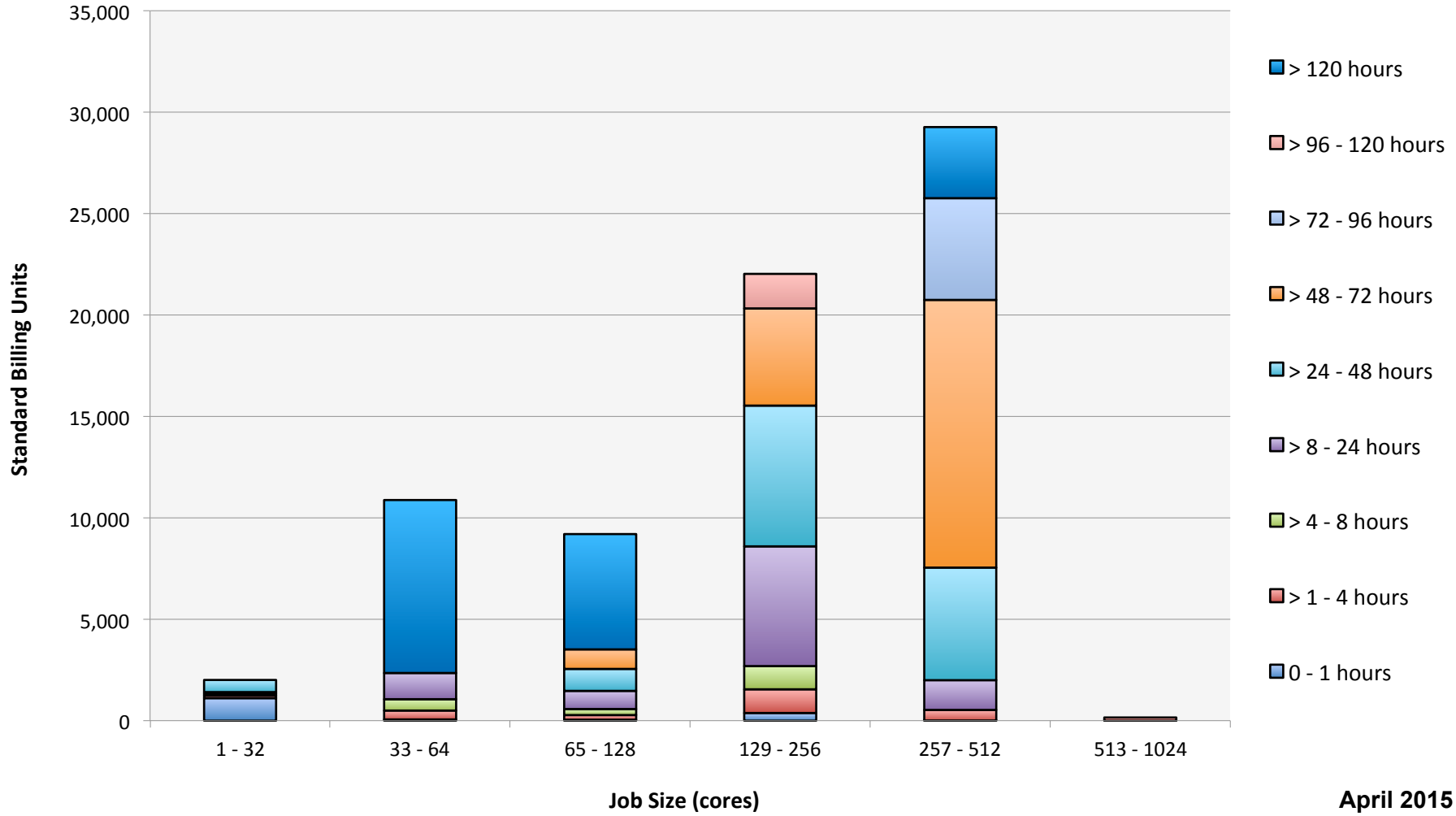
Endeavour:
Monthly Utilization by Job Length



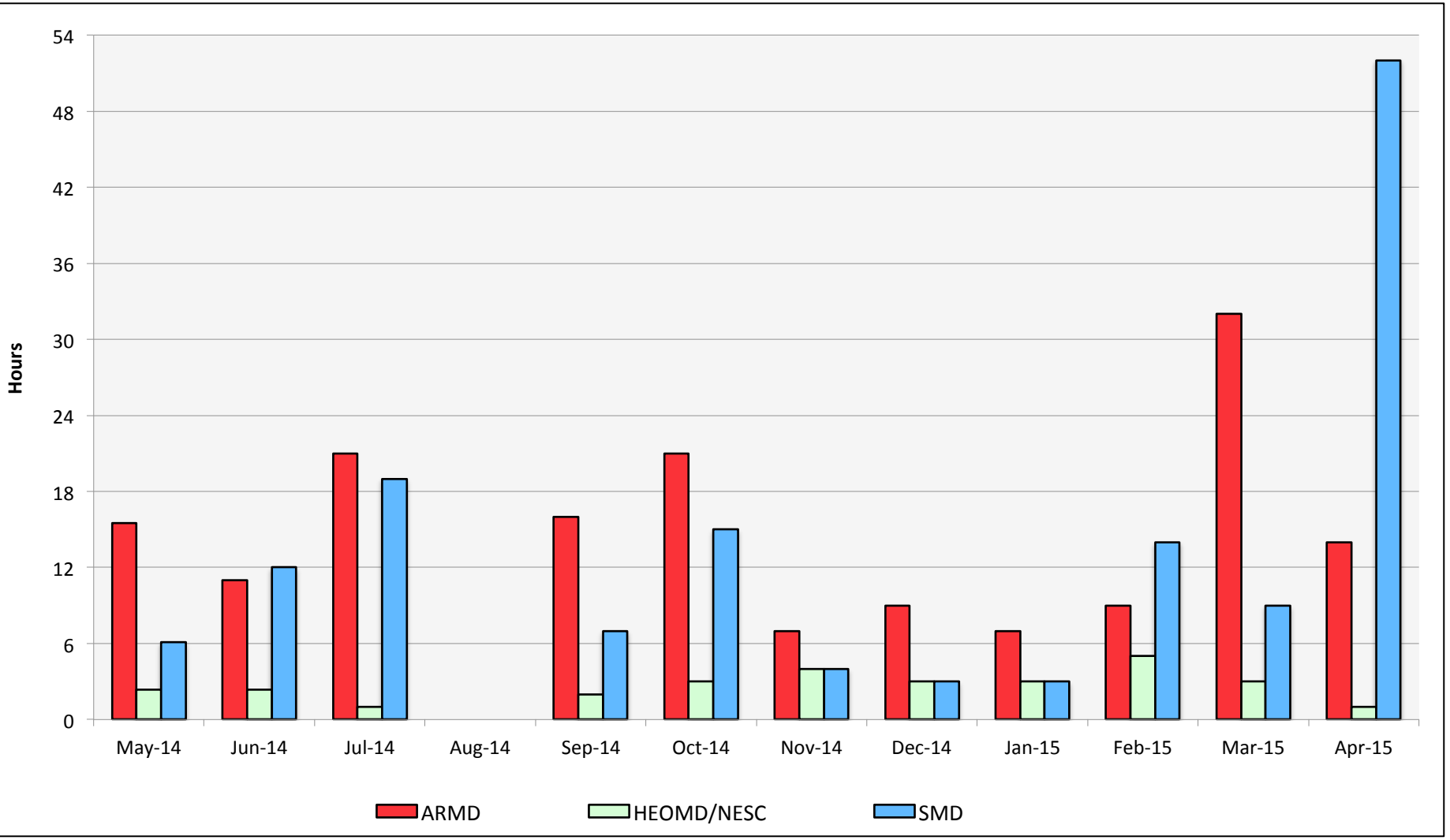
Endeavour:
Monthly Utilization by Size and Mission



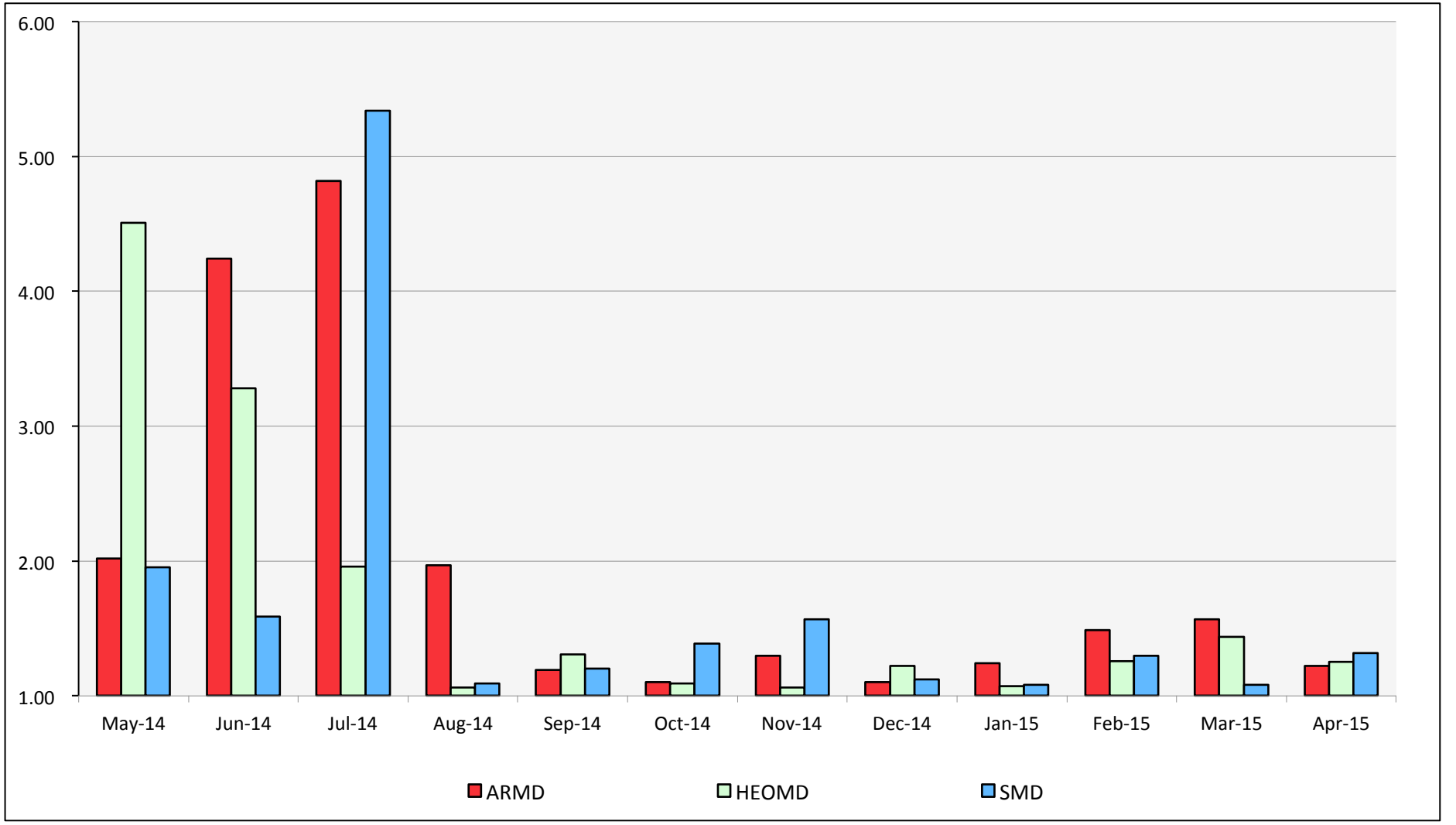
Endeavour:
Monthly Utilization by Size and Length



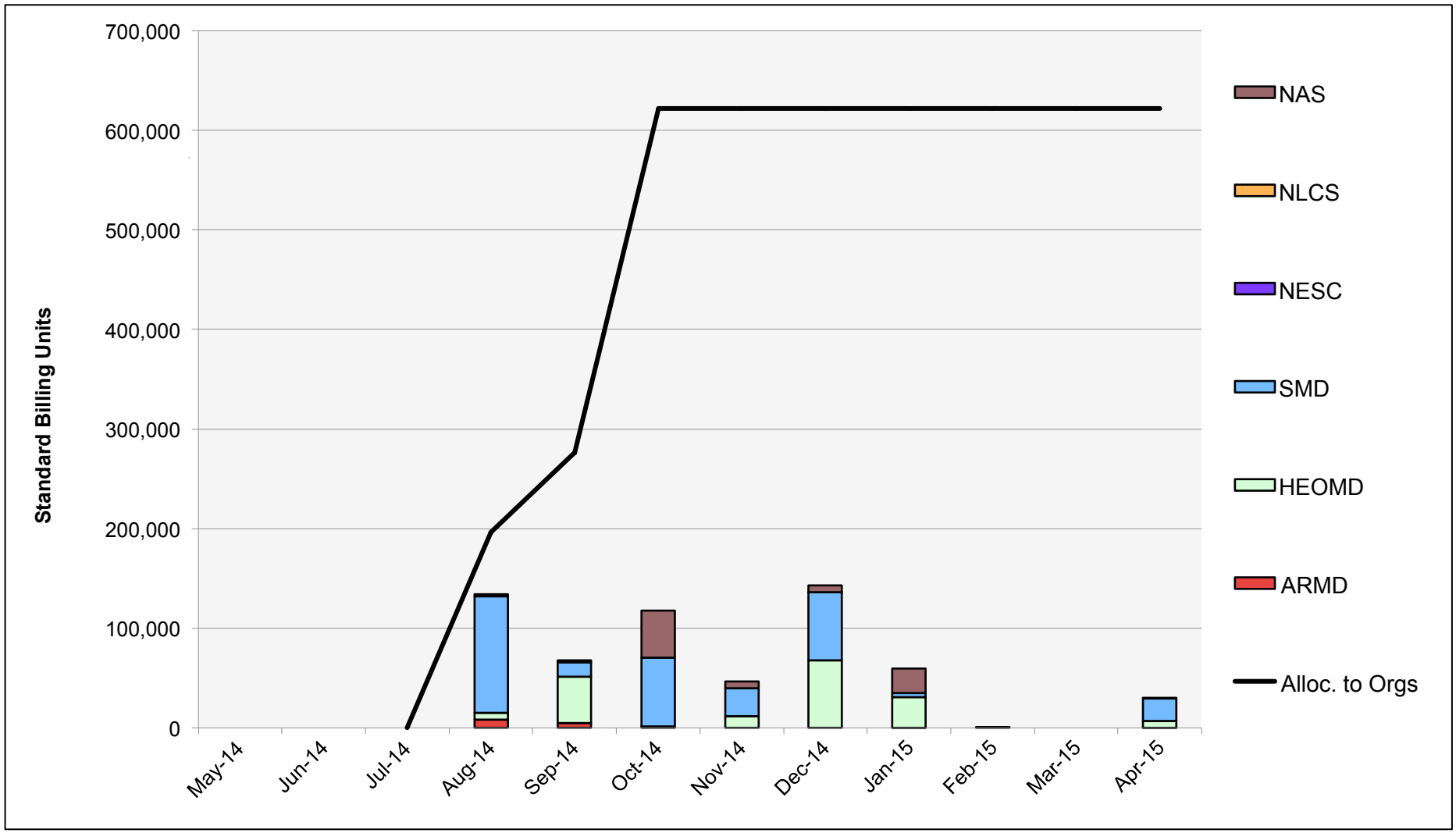
Endeavour:
Average Time to Clear All Jobs



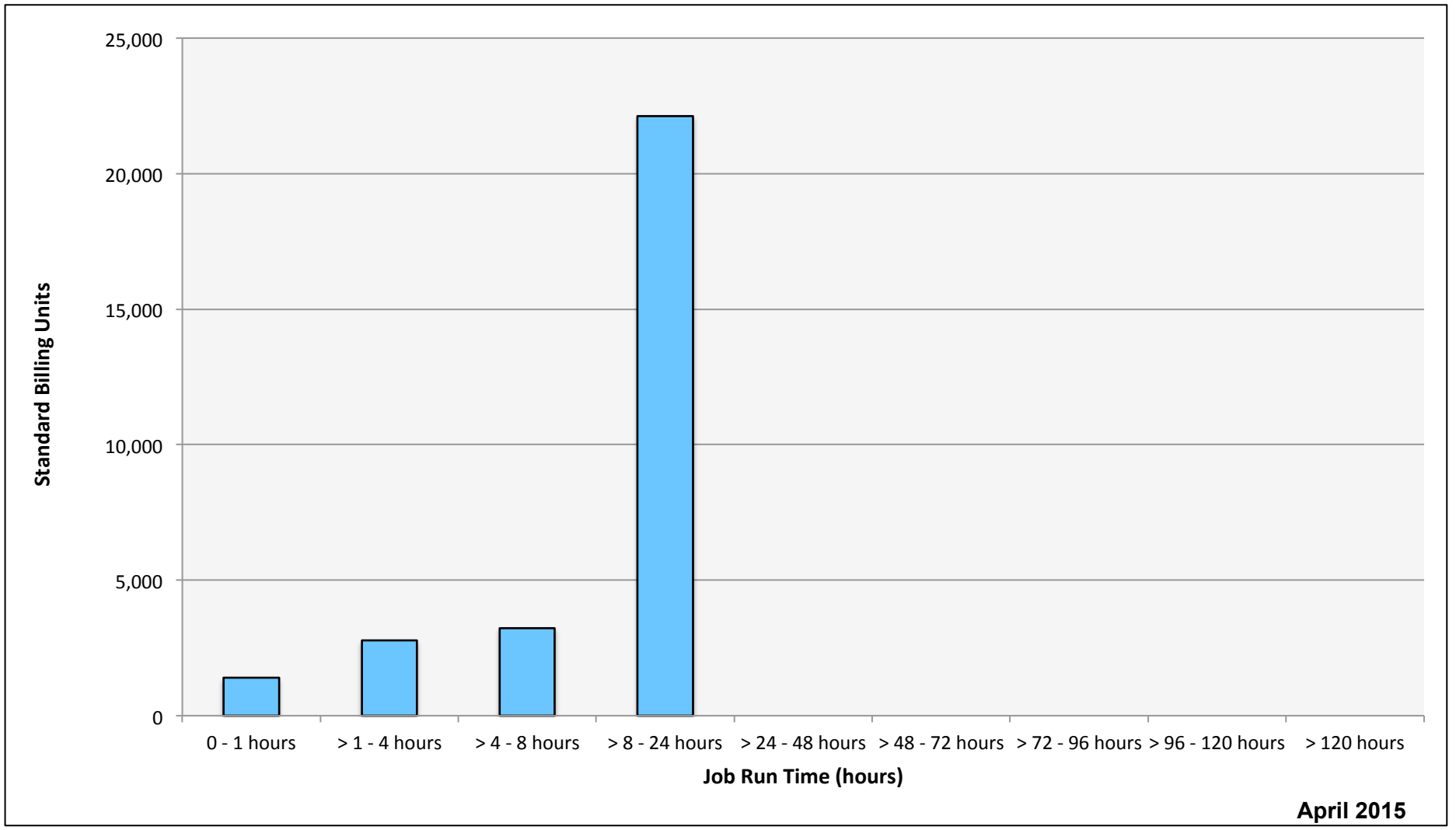
Endeavour:
Average Expansion Factor



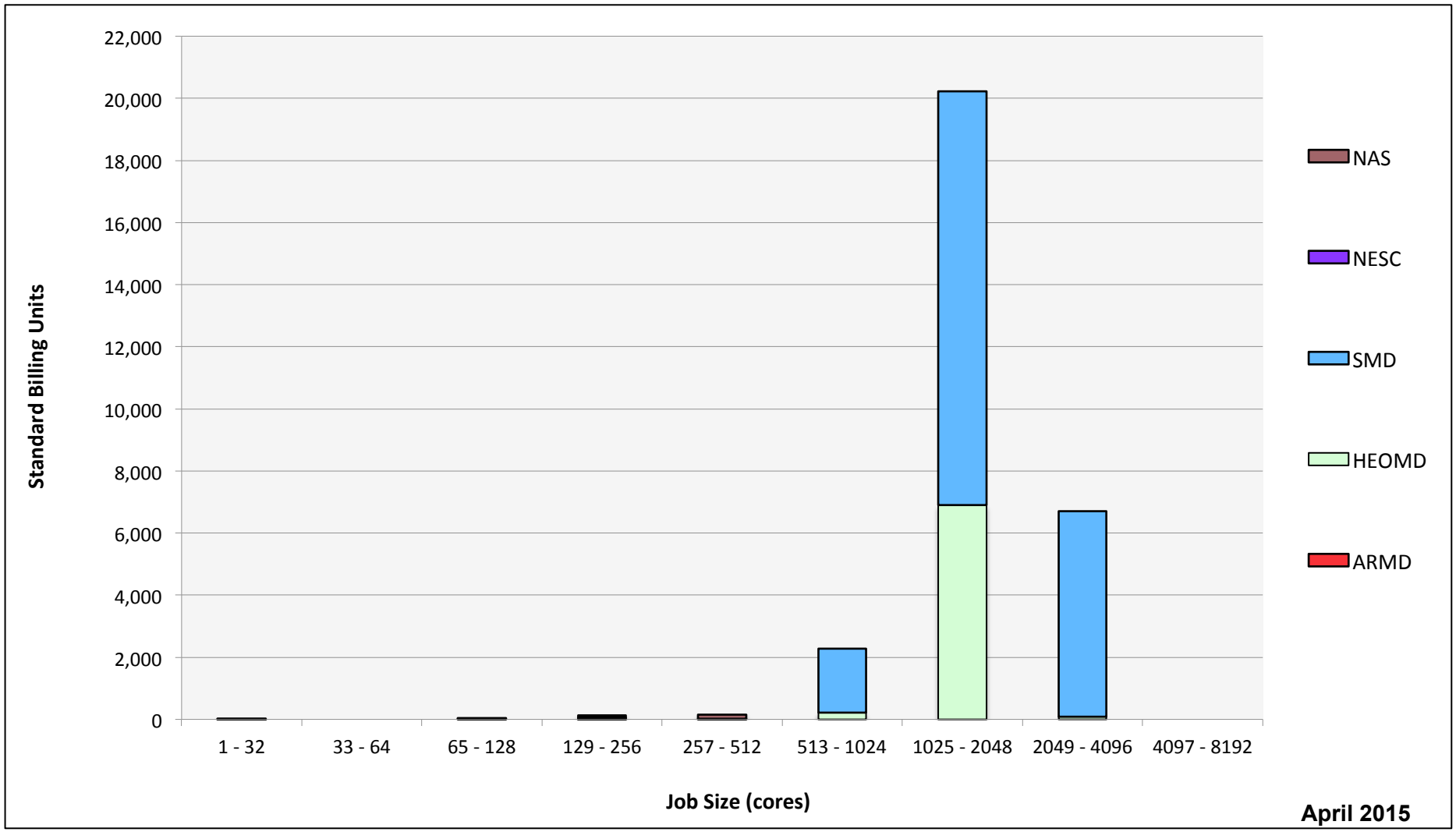
Merope:
SBUs Reported, Normalized to 30-Day Month



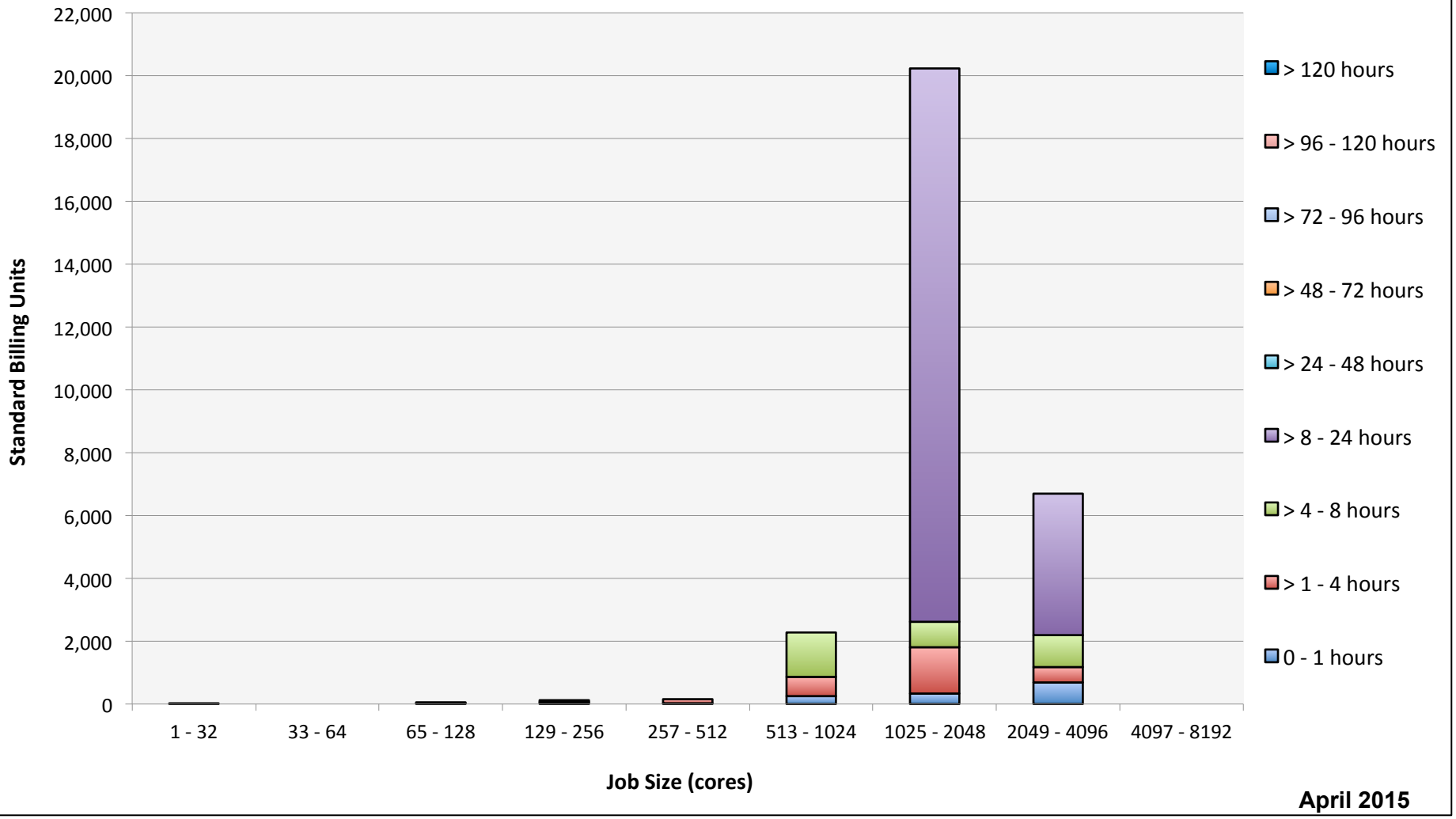
Merope:
Monthly Utilization by Job Length



Merope:
Monthly Utilization by Size and Mission



Merope:
Monthly Utilization by Size and Length



Merope:
Average Expansion Factor