Project Status Report

High End Computing Capability
Strategic Capabilities Assets Program

October 10, 2016

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

Facilities Team Completes Major Milestone for MSF Module Installation

- HECC Facilities engineers, in coordination with NASA Ames (Code J) staff, fulfilled another major milestone for the prototype Modular Supercomputing Facility (MSF) project: the installation of the initial SGI/CommScope module.
- HECC and SGI staff loaded the modular building with 16 SGI compute racks with Intel E5-2680v4 (Broadwell) processors and 2 I/O racks.
- The DCU-20 module is capable of housing 16 racks, and is adiabatically cooled. Water is only required for cooling at ambient temperatures above 85 degrees “wet-bulb” (calculated using temperature and humidity).
- The module was assembled from 15 sections that were forklifted into place, bolted together, and welded to the steel structures embedded in the concrete pad.
- The MSF is scheduled to go into production in December 2016.

Mission Impact: By working closely with Center Operations staff and the construction contractor, the HECC Modular Supercomputing Facility (MSF) project team ensured the successful preparation for and installation of the DCU-20 module for the MSF.

The newly installed SGI/CommScope DCU-20 module, located across the street from the main NASA Advanced Supercomputing facility.

POCs: William Thigpen, william.w.thigpen@nasa.gov, (650) 604-1061, NASA Advanced Supercomputing (NAS) Division;
Chris Tanner, christopher.tanner@nasa.gov, (650) 604-6754, NAS Division, CSRA LLC

Latest Generation of Intel Xeon Phi System Made Available For Testing

- HECC engineers installed an SGI system containing Intel Xeon Phi 7230 (Knights Landing, or KNL) processors, and made it available to testers for evaluation of the characteristics and performance of the new processors.
- The evaluation system consists of 20 nodes containing 64 cores and 192 gigabytes (GB) of memory on each node.
- The system is also equipped with Intel's Omni-Path fabric, an alternative to the InfiniBand (IB) network, which can operate at speeds up to 100 gigabits per second (Gb/s). In comparison, the IB network is capable of speeds up to 56 Gb/s.
- The system is available for staff and early-access users to evaluate the performance and the suitability of the Intel Xeon Phi for NASA codes.
- The evaluation system was procured after initial tests from two loaner nodes looked promising for conducting larger-scale testing of performance across multiple nodes.

Mission Impact: Evaluating leading-edge technology provides real-world data for future procurements that will provide the best solution to meet NASA's high-end computing requirements.

Birds-eye view of the SGI test system, consisting of 20 nodes containing Intel Xeon Phi 7230 (Knights Landing) processors and an administrative management system. The system is a self-contained cluster, but has the capability to interconnect with the Lustre filesystem for future testing.

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 Expands Lustre Filesystem Capacity

- HECC augmented the capacity of the nobackupp1 Lustre filesystem to support the increasing demand for temporary scratch space on Pleiades.
- The filesystem grew by an additional 2.8 petabytes (PB) of raw storage—a 67% increase in capacity.
- The hardware installation was completed during a required two-day downtime of the filesystem.
- The rest of the expansion activity, including configuration and integration of new equipment into the filesystem, was transparent to the users.
- The increase in capacity was funded by the Estimating the Circulation & Climate of the Ocean (ECCO) project to support their growing data requirements on Pleiades.

Mission Impact: HECC's increased storage capacity will enable users to more fully utilize the computing resources and run more data-intensive applications for NASA research projects.

HECC systems engineers relocated Lustre filesystem hardware within existing racks to provide space for the new equipment.

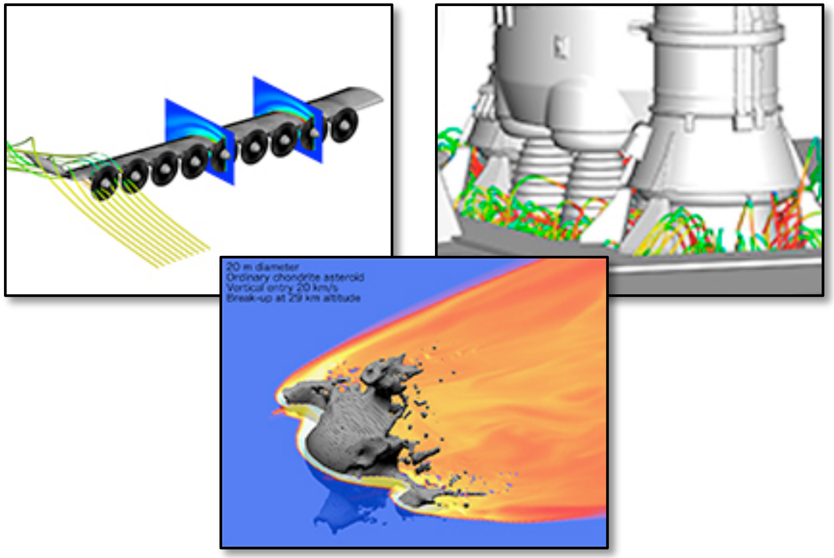
POCs: Bob Ciotti, bob.ciotti@nasa.gov, (650) 604-4408, NASA Advanced Supercomputing (NAS) Division;
Davin Chan, davin.chan@nasa.gov, (650) 604-3613, NAS Division, CSRA LLC.

September 2016 Usage on Pleiades Sets New 30-Day Record of 20.3 Million SBUs

- September usage on the Pleiades supercomputer set a new normalized (30-day-month) record.
- Over 20.3 million Standard Billing Units (SBUs*) were used by NASA's science and engineering organizations, exceeding the previous normalized record of 20.1 million SBUs set in July 2016.
- This increase was enabled by high demand, system stability, and efficient operations that delivered system utilization of over 87% (where 75% utilization is the target).
- Over 325 projects from all across NASA used time on Pleiades during September.
- The top 10 projects used from 415,306 to 1,337,227 SBUs each, 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.*

Mission Impact: Increasing Pleiades' system capacity provides mission directorates with more resources for the accomplishment of their goals and objectives.



Images representing projects on Pleiades from different mission directorates. From top left: (1) Simulation of a distributed electric propulsion concept, *Karen Deere, Sally Viken, NASA/Langley.* (2) Simulation of potential debris trajectories from various parts of the launch pad and SLS structures, *Brandon Williams, NASA/Marshall, Jacobs ESSSA Group.* (3) Simulation of an asteroid breaking up during atmospheric entry, *Darrel Robertson, NASA/Ames, Science & Technology Corp.*

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

ESS Team Completes Deployment of Mac OS X 10.11 to Staff Workstations

- HECC's Engineering Servers and Services (ESS) team completed the deployment of Mac OS X 10.11 (El Capitan) to 185 workstations and laptops used by staff at the NAS facility.
- The ESS team began the rollout in May, after the Ames Security team approved the El Capitan image.
- Development of the El Capitan rollout included:
  - Building the NAS image using Casper.
  - Configuring security and FileVault.
  - Configuring Centrify for smart card authentication.
  - Testing and upgrading scientific software as needed.
  - Completing full backups, system upgrades, and final checks on each upgraded system.
- Using knowledge gained from the El Capitan upgrade, ESS has begun to evaluate the new macOS Sierra (version 10.12) release.

Mission Impact: Deployment of the Mac OS X 10.11 (El Capitan) image with Centrify smart card authentication enables HECC to take advantage of the latest Apple software and hardware features for our scientific users.

With HECC's completion of the El Capitan upgrade, work has already begun on development of its successor, macOS Sierra.

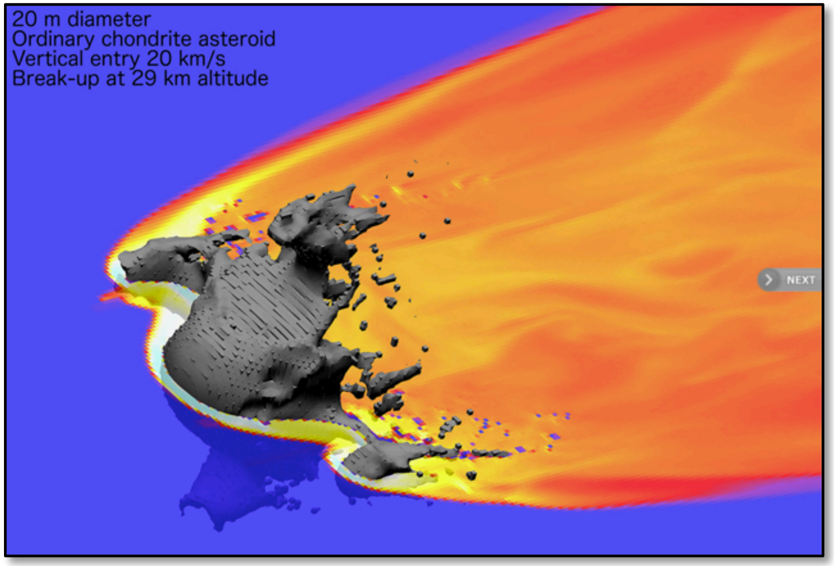
POCs: Ted Bohrer, theodore.w.bohrer@nasa.gov, (650) 604-4335, Ed Garcia, edmund.a.garcia@nasa.gov, (650) 604-1338, NASA Supercomputing Division, ADNET Systems

Using Modeling and Simulation to Predict Damage from an Asteroid Strike on Earth *

- Researchers are running computational fluid dynamics simulations on Pleiades to determine the fragmentation and blast propagation that occurs when asteroids impact the atmosphere or the ground.
  - Simulations of the 2013 asteroid strike over the Russian city of Chelyabinsk, using a simple strength model of the asteroid's rock mass, show that the rock fractures when it hits the stratosphere.
  - Fragmentation and deceleration in the atmosphere produce energy deposition rates very similar to those shown in dashboard camera videos of the event.
  - Propagating the resulting blast wave to the ground produces damage very similar to observations of broken window patterns.
- Simulations of different sizes, speeds, entry angles, and types of asteroids are being used to map out the damage zones for possible impact scenarios, including earthquakes and tsunamis.
- The simulations will be used as part of NASA's Asteroid Threat Assessment Project to provide information that decision makers can use for future characterization and observation efforts, and for mitigation strategies.

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

Mission Impact: This work supports NASA's Grand Challenge initiative focusing on detecting, characterizing, and developing mitigation strategies to defend against potentially life-threatening asteroid strikes.



Simulation of an asteroid breaking up during atmospheric entry. The entry velocity of 20 kilometers per second creates a hot, high-pressure shock wave around the asteroid that causes it to rapidly fragment and burn up. Larger asteroids can survive all the way to the ground where they will create a large crater. *Darrel Robertson, NASA/Ames*

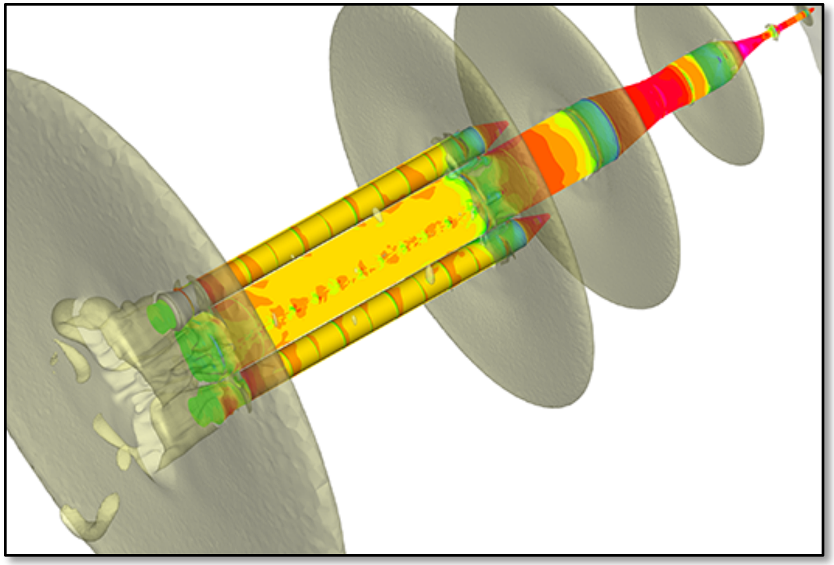
POC: Darrel Robertson, darrel.k.robertson@nasa.gov, (650) 604-1331, NASA Advanced Supercomputing Division, Science and Technology Corp.

Simulations Run on Pleiades Accurately Predict Buffet as SLS Nears the Speed of Sound *

- Aerospace research engineers at NASA Langley performed detailed Space Launch System flow field analyses to model flow-induced vibratory loads on the vehicle during ascent flight nearing the speed of sound.
- The team ran delayed detached eddy simulations on Pleiades to compute the unsteady flow around the full vehicle, monitoring surface-pressure time histories at over 600 locations.
- Comparison of computational fluid dynamics (CFD) results with wind tunnel data showed good agreement. The team found that:
  - Location of the peak oscillatory force was the same for both methods.
  - Data analyses with histograms indicated the simulations captured the physical phenomenon in the flow field.
  - Large-scale simulations of 0.5 to 1 second in duration were needed to acquire sufficient data to converge frequency content.
- The availability of HECC resources allowed for a timely turnaround of data, which increases the viability of CFD simulations as part of the design process of existing and future vehicles.

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

Mission Impact: The large capacity of the Pleiades supercomputer enabled researchers at NASA Langley to obtain computational data for the safe design of the SLS at an order of magnitude faster than using mid-range computers.



Surface pressure coefficient (colored magenta to blue) with sonic isosurfaces (grey disks), from a computation of the transonic flow around the Space Launch System (SLS) configuration. Variations in pressure along the body of the SLS can be seen, particularly around the protuberances on the smoother surface of the vehicle.

POCs: Stephen Alter, stephen.j.alter@nasa.gov, (757) 864-7771, Greg Brauckmann, gregory.j.brauckmann@nasa.gov, (757) 864-5234, NASA Langley Research Center

HECC Facility Hosts Several Visitors and Tours in September 2016

- HECC hosted 9 tour groups in September; guests learned about the agency-wide missions being supported by HECC assets, and some groups also viewed the D-Wave 2X quantum computer system. Tours were limited this month due to a facility shutdown. Visitors this month included:
  - Elżbieta Bieńkowska, European Commissioner (EC). She is responsible for EC/EU programs such as Galileo and Copernicus.
  - A group of military alumni from the Armed Forces Air Intelligence Training Center.
  - Members of NASA's Ad-Hoc Big Data Task Force.
  - Members of the NASA Engineering Standards Panel (NESP), who held their annual face-to-face meeting at NASA Ames.
  - Byonghoon Chong, a visiting IT engineer from the Korea Aerospace Research Institute;
  - Kevin Gallagher, United States Geological Survey (USGS) Associate Director. Gallagher oversees the USGS Geologic and Topographic Mapping, Geological and Geophysical Data Preservation, Biological Information, and Science Informatics programs, as well as the world's largest Earth Science Library.
  - Mitchell Bingemann, science and technology reporter for one of Australia's largest daily newspapers, *The Australian*.

NAS Division Branch Chief Cetin Kiris presents computational fluid dynamic results on the NAS mini-hyperwall to the members of the NASA Engineering Standards Panel.

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

Papers

- "**Volume-Rendering on a 3D hyperwall: A Molecular Visualization Platform for Research, Education, and Outreach**," P. MacDougall, C. Henze, A. Volkov, Journal of Molecular Graphics and Modeling, Vol. 70, November 2016, published online September 5, 2016. *
  http://www.sciencedirect.com/science/article/pii/S109332631630167X
- "**UV Absorption Line Ratios in Circumgalactic Medium at Low Redshift in Realistic Cosmological Hydrodynamic Simulations**," R. Cen, M. Safarzadeh, arXiv:1609.03583 [astro-ph.GA], September 12, 2016. *
  https://arxiv.org/abs/1609.03583
- "**The Emergence of Solar Supergranulation as a Natural Consequence of Rotationally-Constrained Interior Convection**," N. Featherstone, B. Hindman, arXiv: 1609:05153 [astro-ph.SR], September 12, 2016. *
  https://arxiv.org/abs/1609.05153
- "**The Effect of Representing Bromine from VSLS on the Simulation and Evolution of Antarctic Ozone**," L. Oman, et al., Geophysical Research Letters (Early View), September 19, 2016. *
  http://onlinelibrary.wiley.com/doi/10.1002/2016GL070471/full
- "**Reflected Charged Particle Populations Around Dipolar Lunar Magnetic Anomalies**," J. Deca, A. Divin, The Astrophysical Journal, Vol. 829, No. 2, September 22, 2016. *
  http://iopscience.iop.org/article/10.3847/0004-637X/829/2/60/meta

Papers (cont.)

- "**High-Frequency Instabilities of Stationary Crossflow Vorticies in a Hypersonic Boundary Layer**," F. Li, M. Choudhari, P. Paredes, L. Duan, Physical Review Fluids, September 26, 2016. *
http://journals.aps.org/prfluids/abstract/10.1103/PhysRevFluids.1.053603
- "**Simulations of Magnetic Fields in Tidally-Disrupted Stars**," J. Guillochon, M. McCourt, arXiv:1609.08160 [astro-ph.HE], September 26, 2016. *
https://arxiv.org/abs/1609.08160
- "**No Conclusive Evidence for Transits of Proxima b in MOST Photometry**," D. Kipping, et al., arXiv:1609.08718 [astro-ph.EP], September 28, 2016. *
https://arxiv.org/abs/1609.08718
- "**Microscopic Processes in Global Relativistic Jets Containing Helical Magnetic Fields**," K.-I. Nishikawa, et al., *Galaxies*, Vol. 4, September 29, 2016. *
http://www.mdpi.com/2075-4434/4/4/38/htm

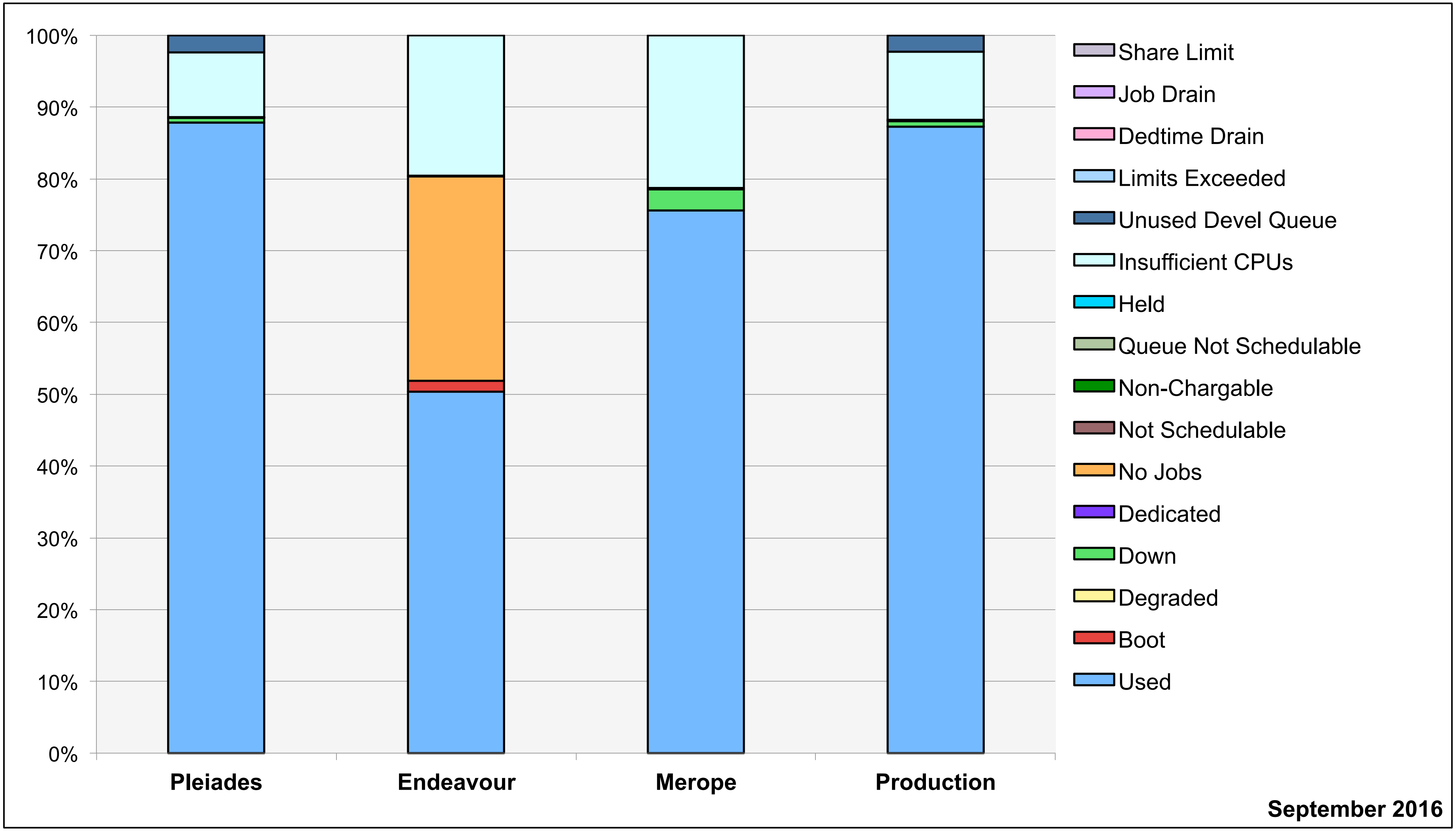
Presentations

- "**HECC – Moving to the Future Today**," W. Thigpen, Keynote Presentation at the Data Center Dynamics Converged Conference, Mexico City, Mexico, September 27-28, 2016.
- "**NASA Big Data Challenges: Ames Perspective**," P. Mehrotra, NASA's Ad-Hoc Big Data Task Force Meeting, NASA Ames, Moffett Field, CA, September 28-30, 2016.
- "**NASA Earth Exchange: Helping Scientists Tackle Big Data**," R. Nemani, P. Votava and S. Ganguly, NASA's Ad-Hoc Big Data Task Force Meeting, NASA Ames, Moffett Field, CA, September 28-30, 2016.
- "**Securing NASA's Most Powerful Supercomputer**," T. Hinke, presented at the National Strategic Computing Initiative (NSCI) High-Performance Computing Security Workshop, Gaithersburg, MD, September 29-30, 2016.
- "**NASA Advanced Computing Environment for Science & Engineering**," R. Biswas, Invited Presentation at the 63rd HPC User Forum, Oxford, UK, September 29–30, 2016.

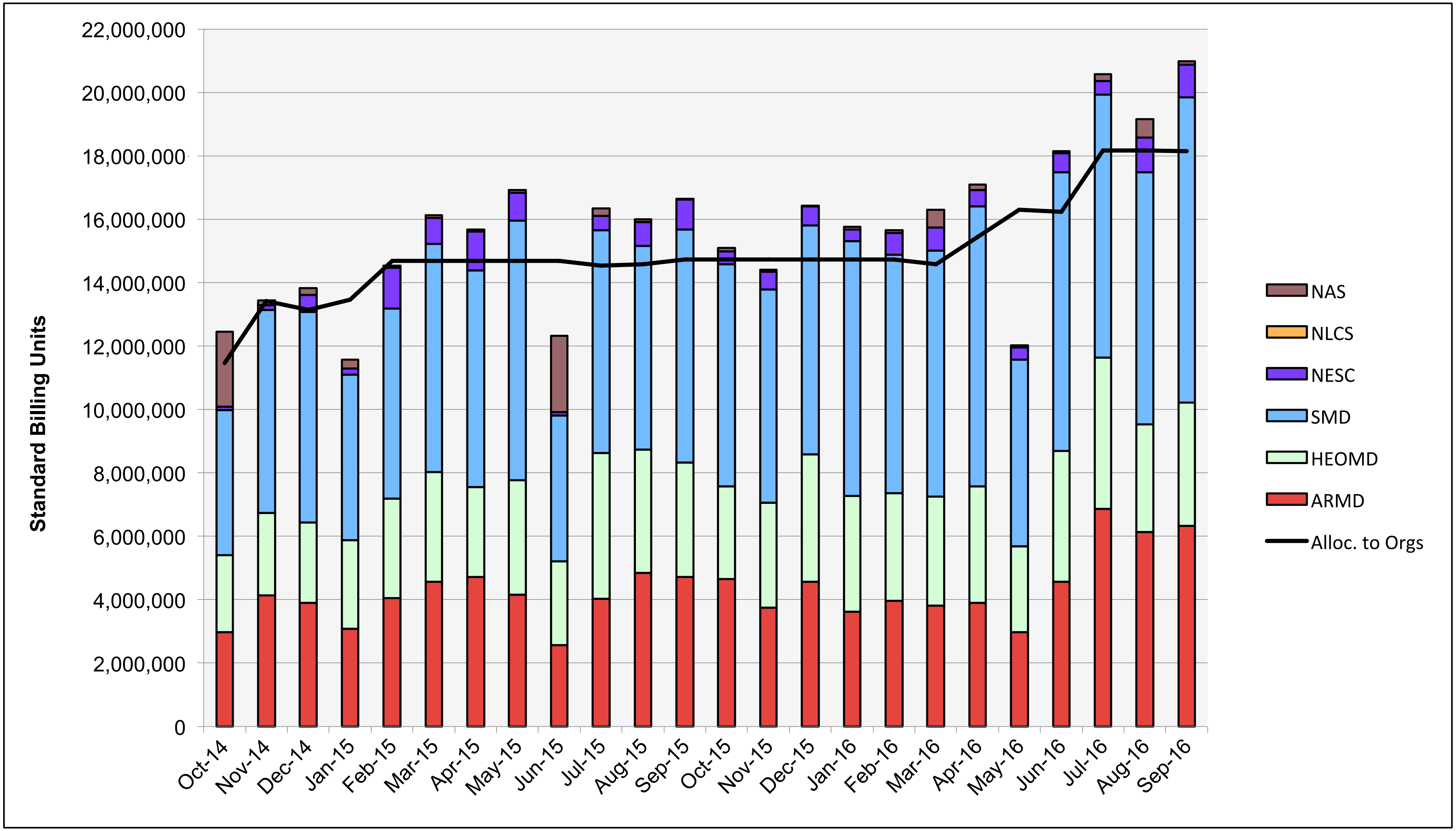
News and Events

- **Galactic Fireworks Illuminate Monster Hydrogen Blob**, *National Radio Astronomy Observatory*, September 21, 2016—An international team of researchers using the Atacama Large Millimeter/submillimeter Array and other telescopes has discovered the power source illuminating a so-called Lyman-alpha Blob—a rare, brightly glowing, and enormous concentration of gas in the distant universe. Simulations were run on the NAS facility's Pleiades supercomputer.
https://public.nrao.edu/news/pressreleases/2016-lyman-alpha-alma
  - **Giant Green Space Blob Mystery Solved**, *Space.com*, September 21, 2016.
  http://www.space.com/34130-giant-green-space-blob-mystery-solved.html
  - **ALMA Uncovers Secrets of Giant Space Blob**, *ALMA Observatory*, September 21, 2016.
  http://www.almaobservatory.org/en/press-room/press-releases/1038-alma-uncovers-secrets-of-giant-space-blob
  - **Researchers Uncover Secrets of Giant Space Blob**, *Space Ref*, September 21, 2016.
  http://spaceref.com/astronomy/researchers-uncover-secrets-of-giant-space-blob.html

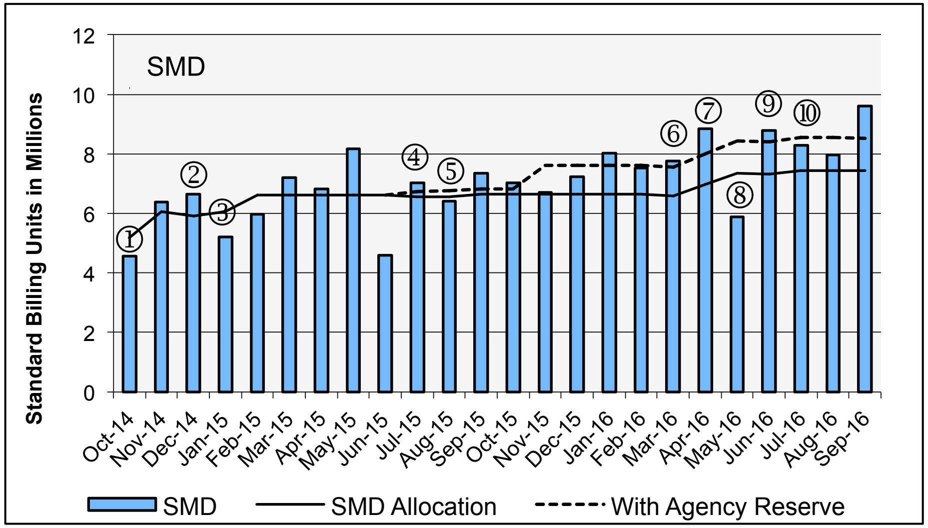
HECC Utilization

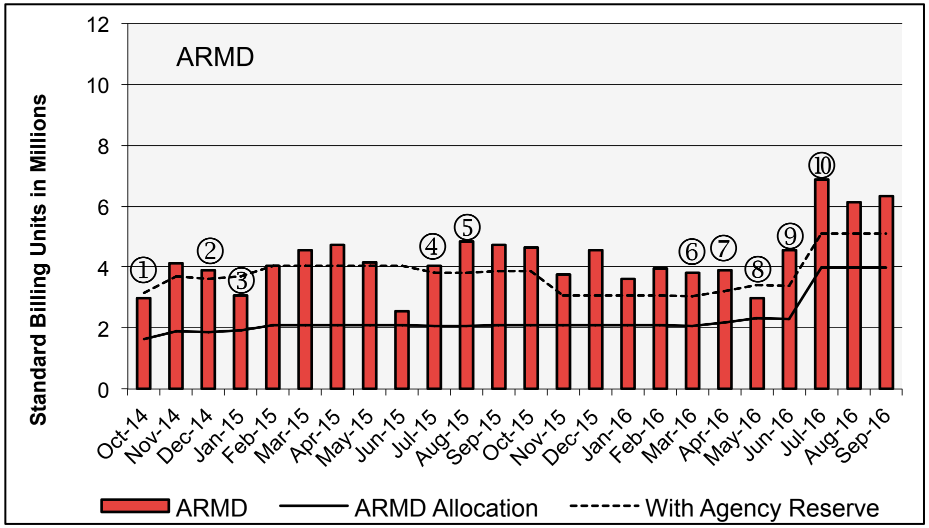


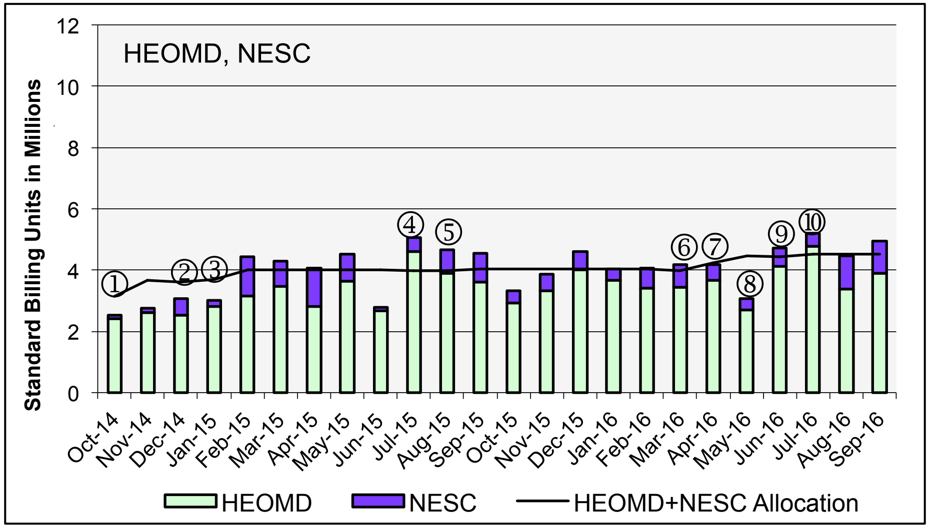
HECC Utilization Normalized to 30-Day Month



HECC Utilization Normalized to 30-Day Month

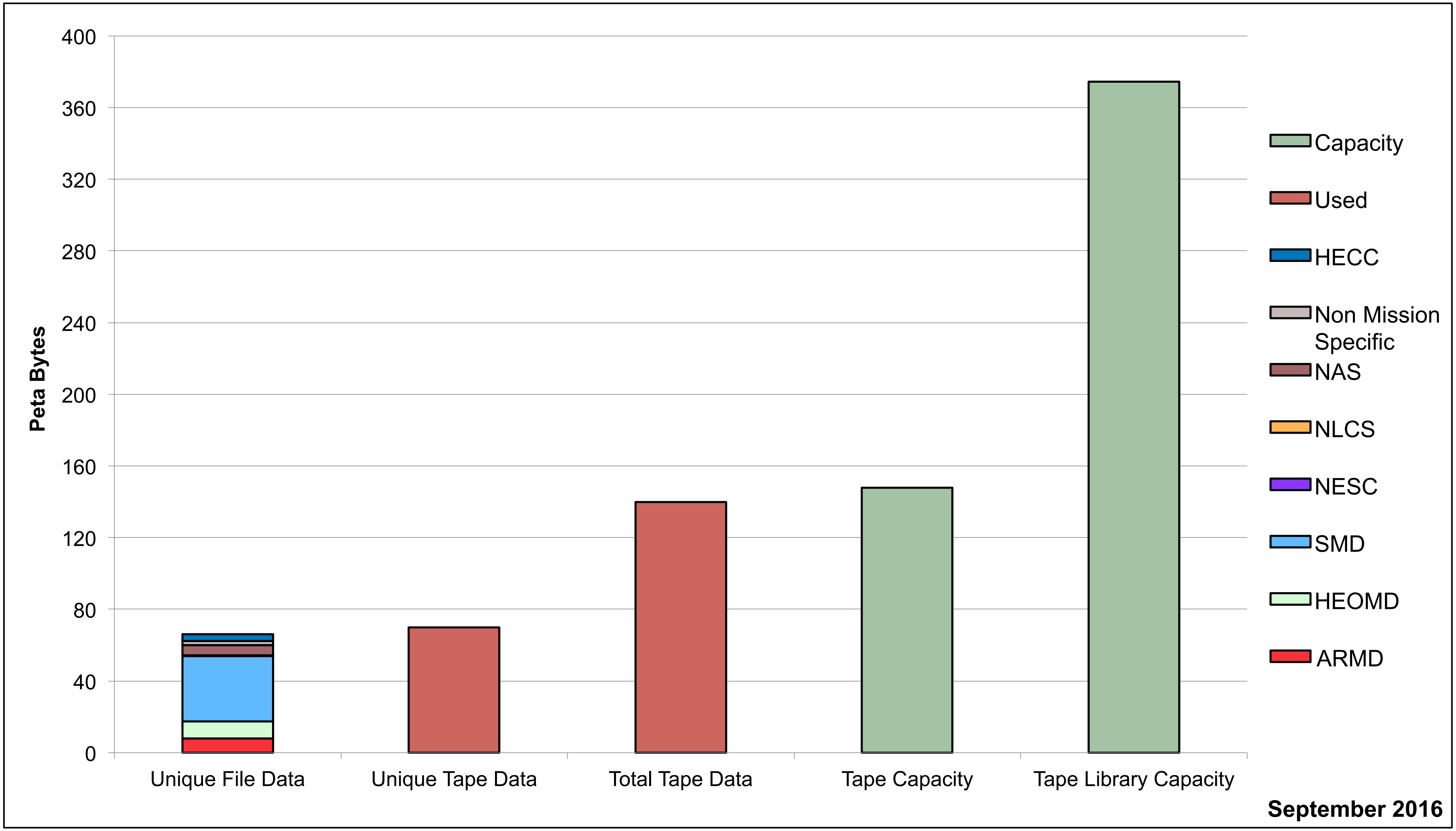




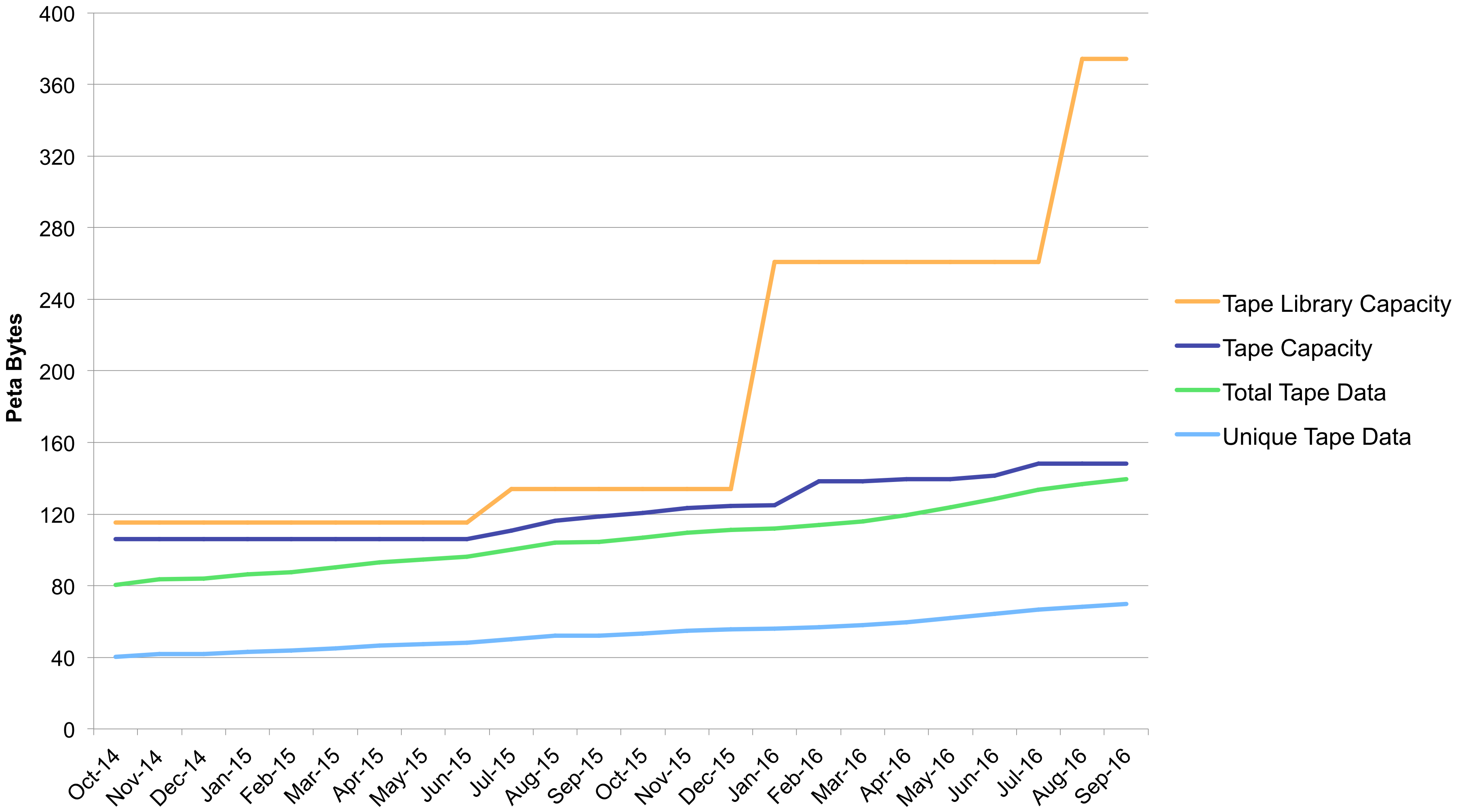


① 16 Westmere racks retired from, 3 Ivy Bridge and 15 Haswell racks added to Pleiades; 10 Nehalem and 2 Westmere racks added to Merope
② 16 Westmere racks retired from Pleiades
③ 14 Haswell racks added to Pleiades
④ 7 Nehalem ½ racks retired from Merope
⑤ 7 Westmere ½ racks added to Pleiades
⑥ 16 Westmere racks retired from Pleiades
⑦ 10 Broadwell racks added to Pleiades
⑧ 4 Broadwell racks added to Pleiades
⑨ 14 (all) Westmere racks retired from Pleiades
⑩ 14 Broadwell racks added to Pleiades (10.5 Dedicated to ARMD)

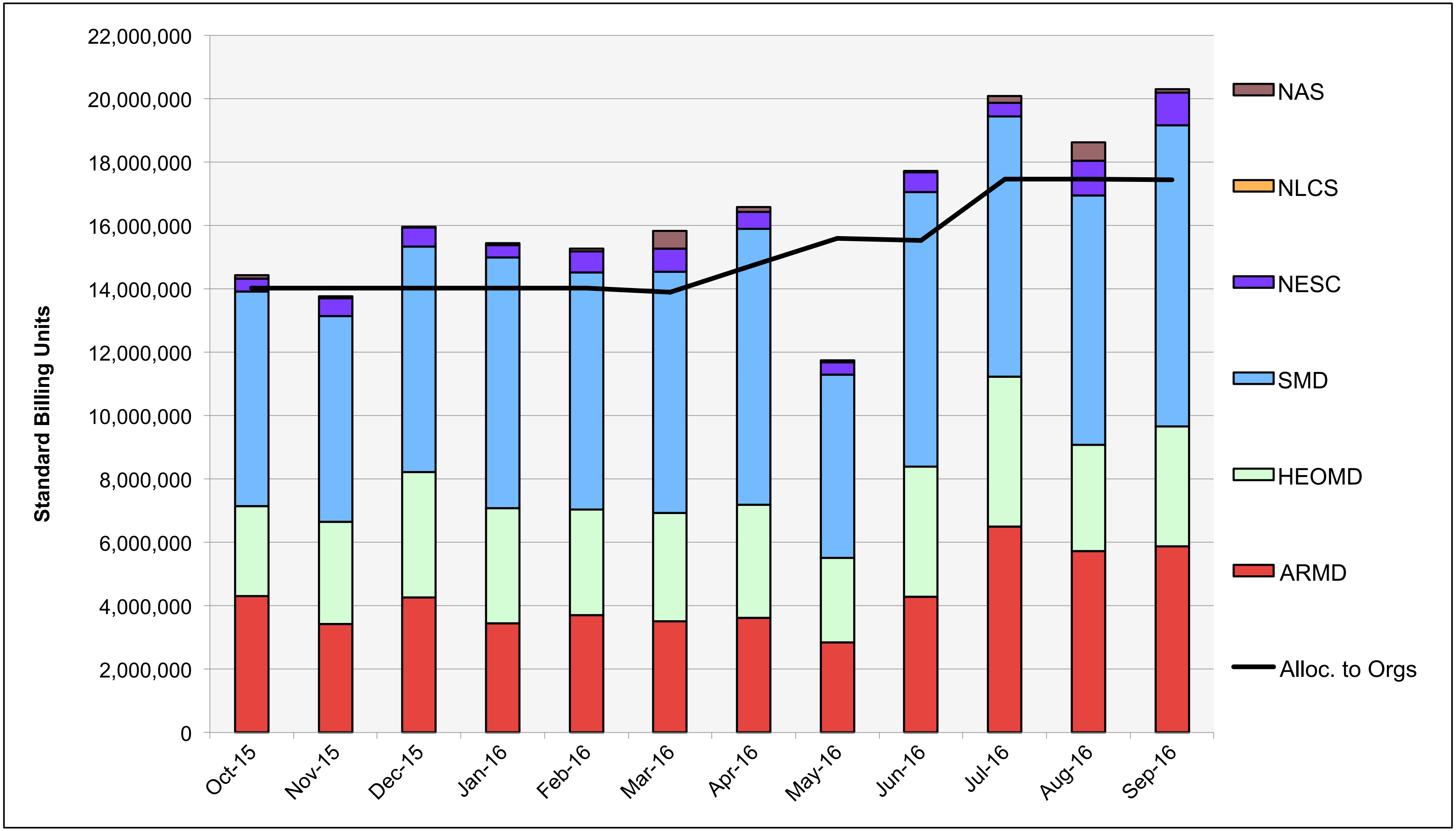
Tape Archive Status



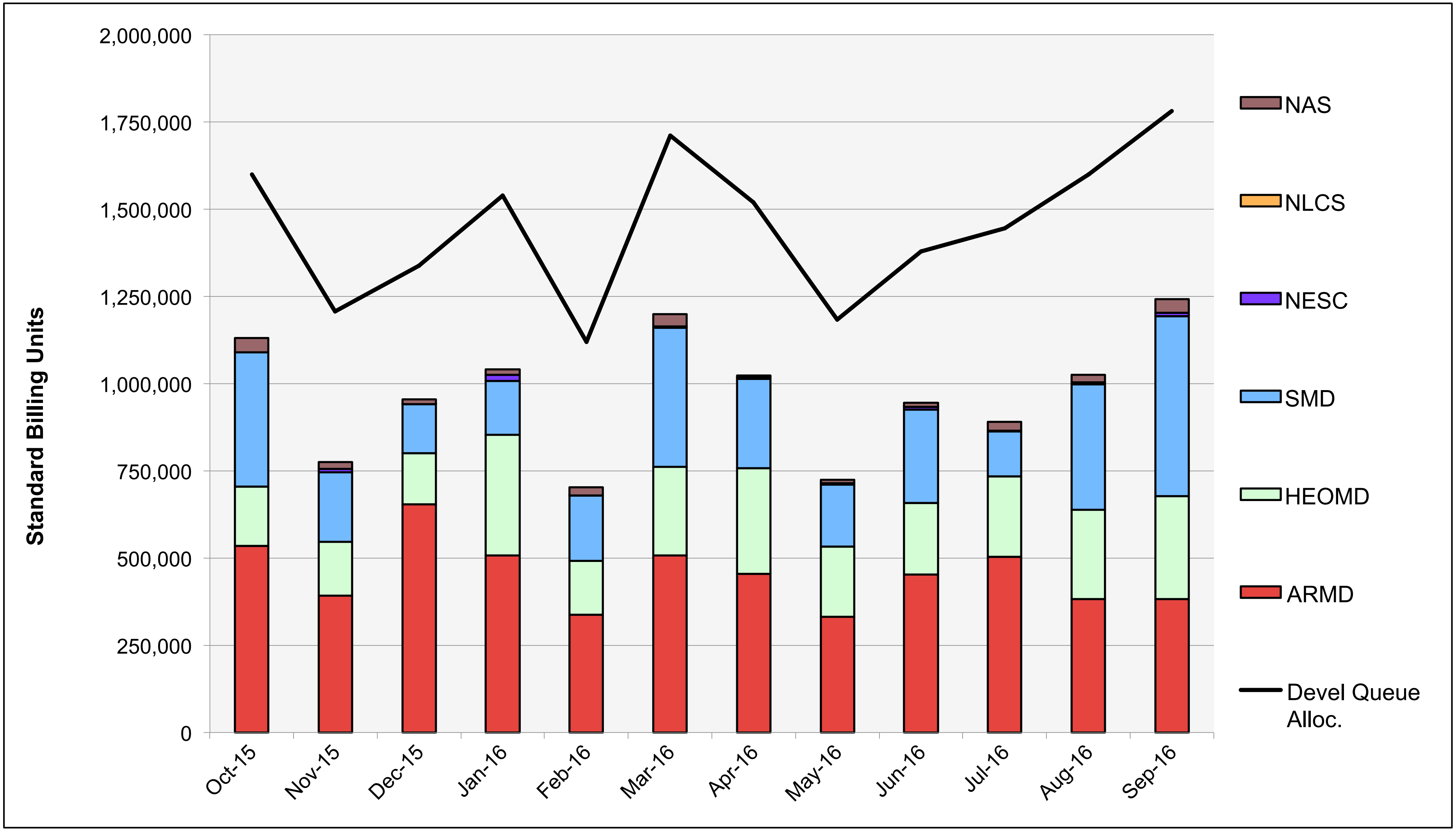
Tape Archive Status



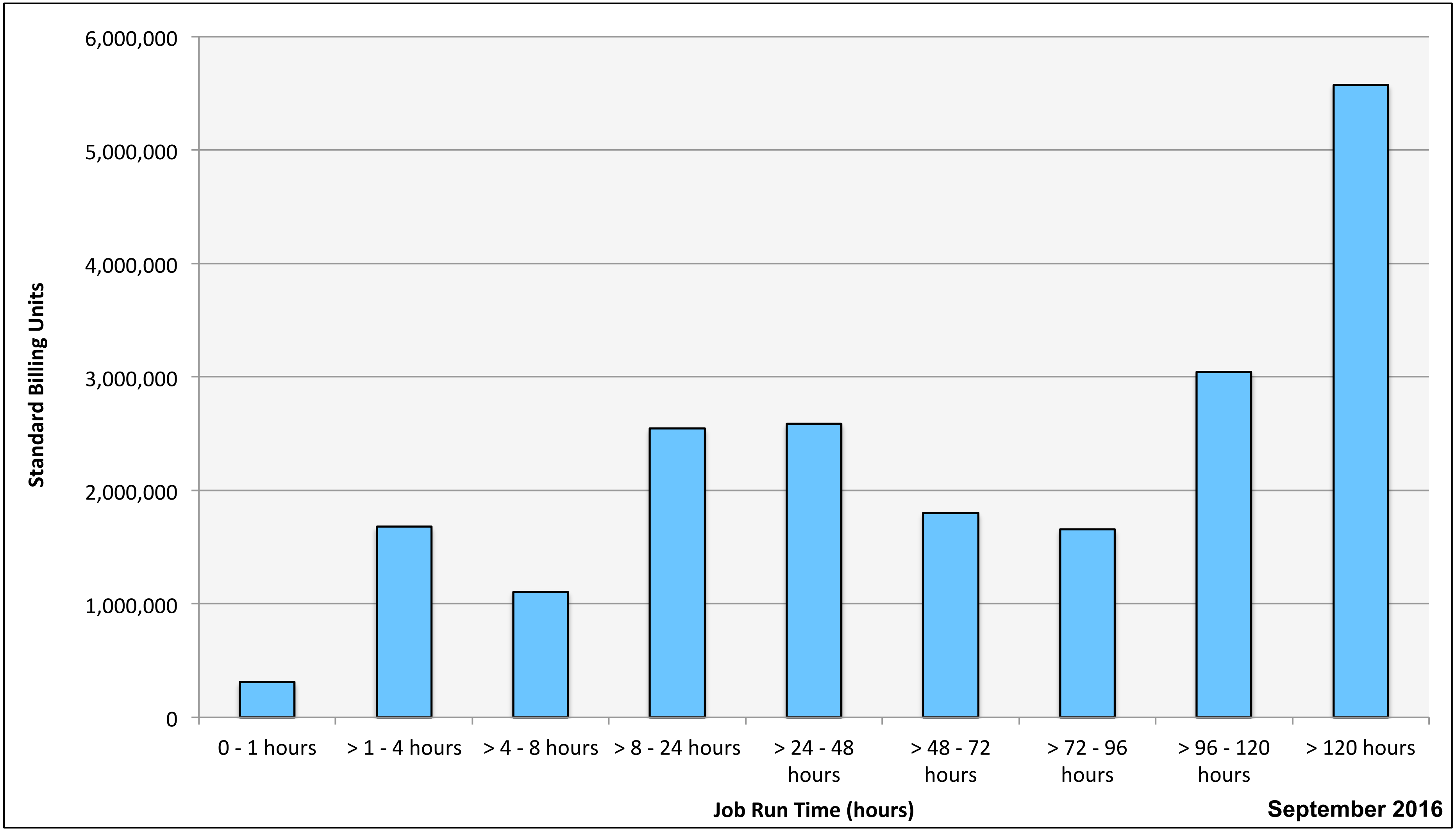
Pleiades:
SBUs Reported, Normalized to 30-Day Month



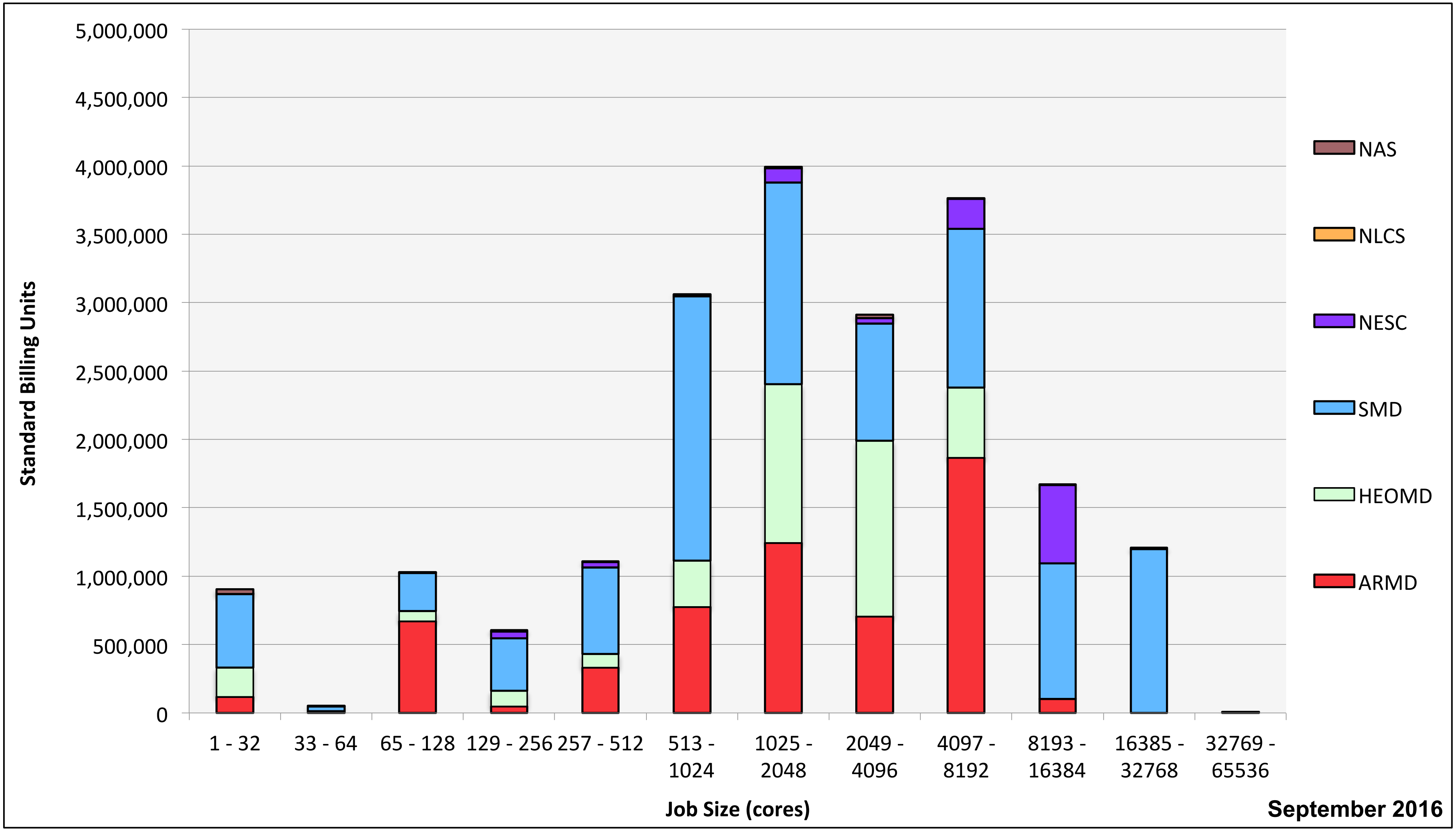
Pleiades: Devel Queue Utilization



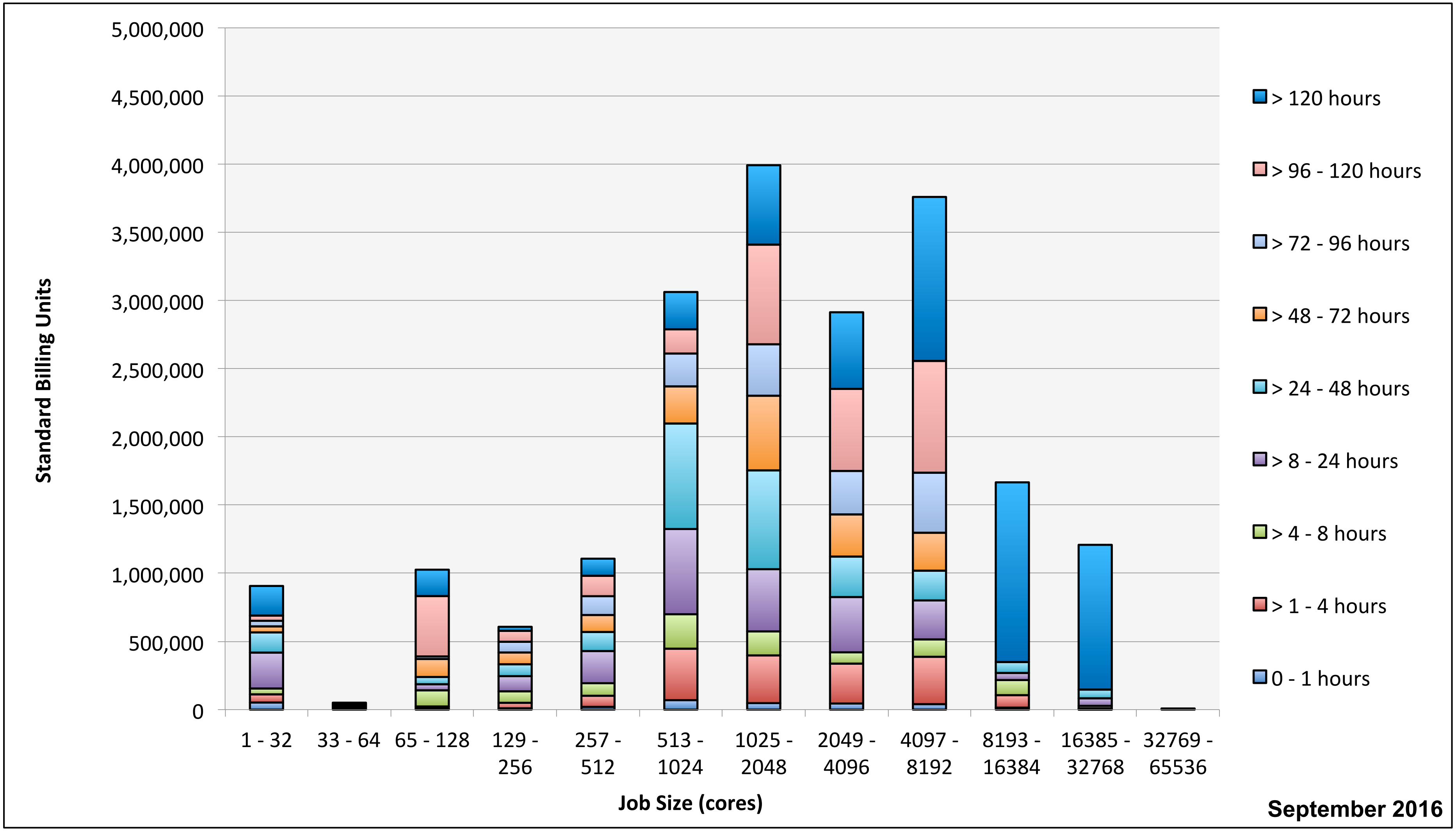
Pleiades:
Monthly Utilization by Job Length



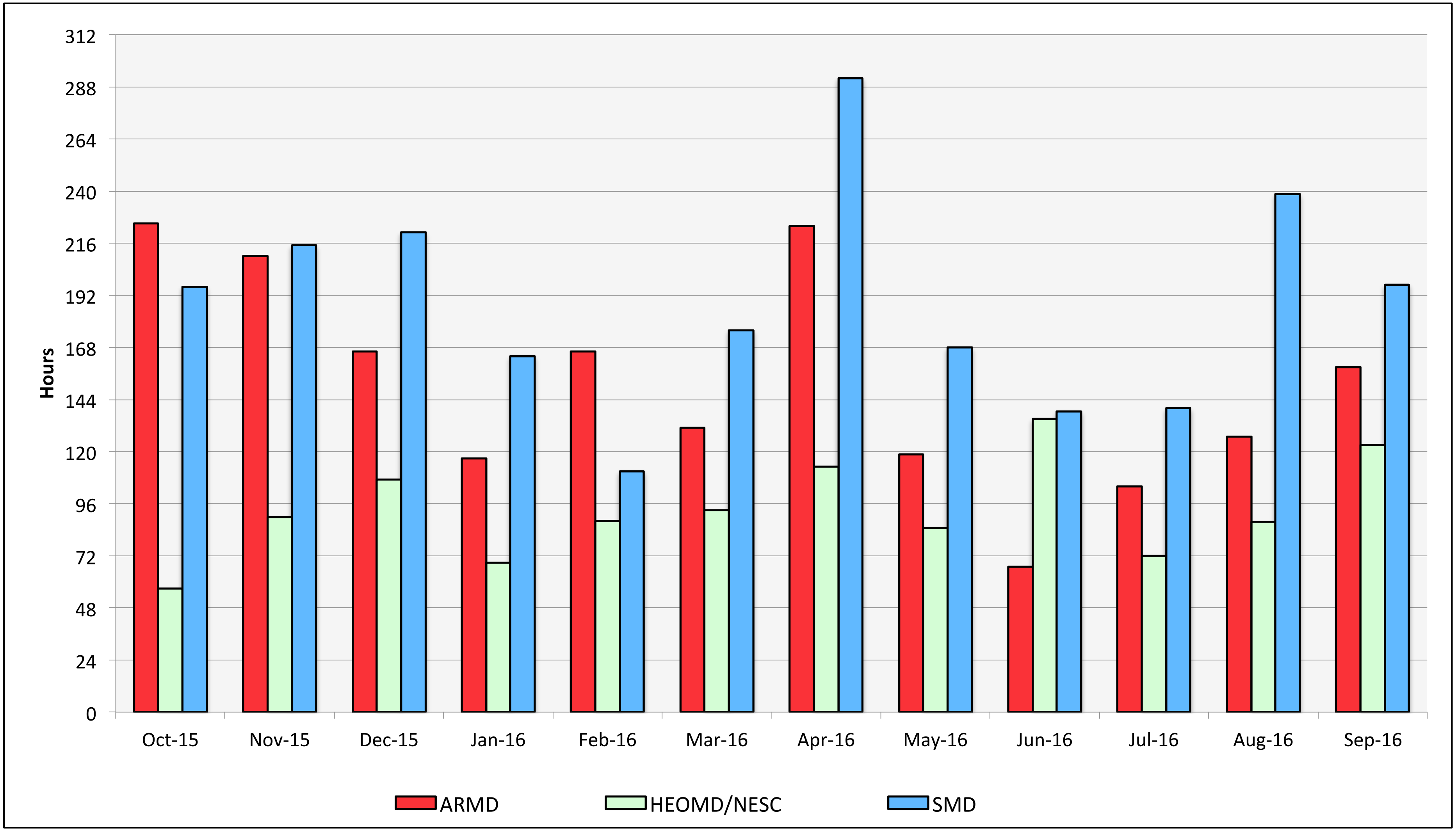
Pleiades: Monthly Utilization by Size and Mission



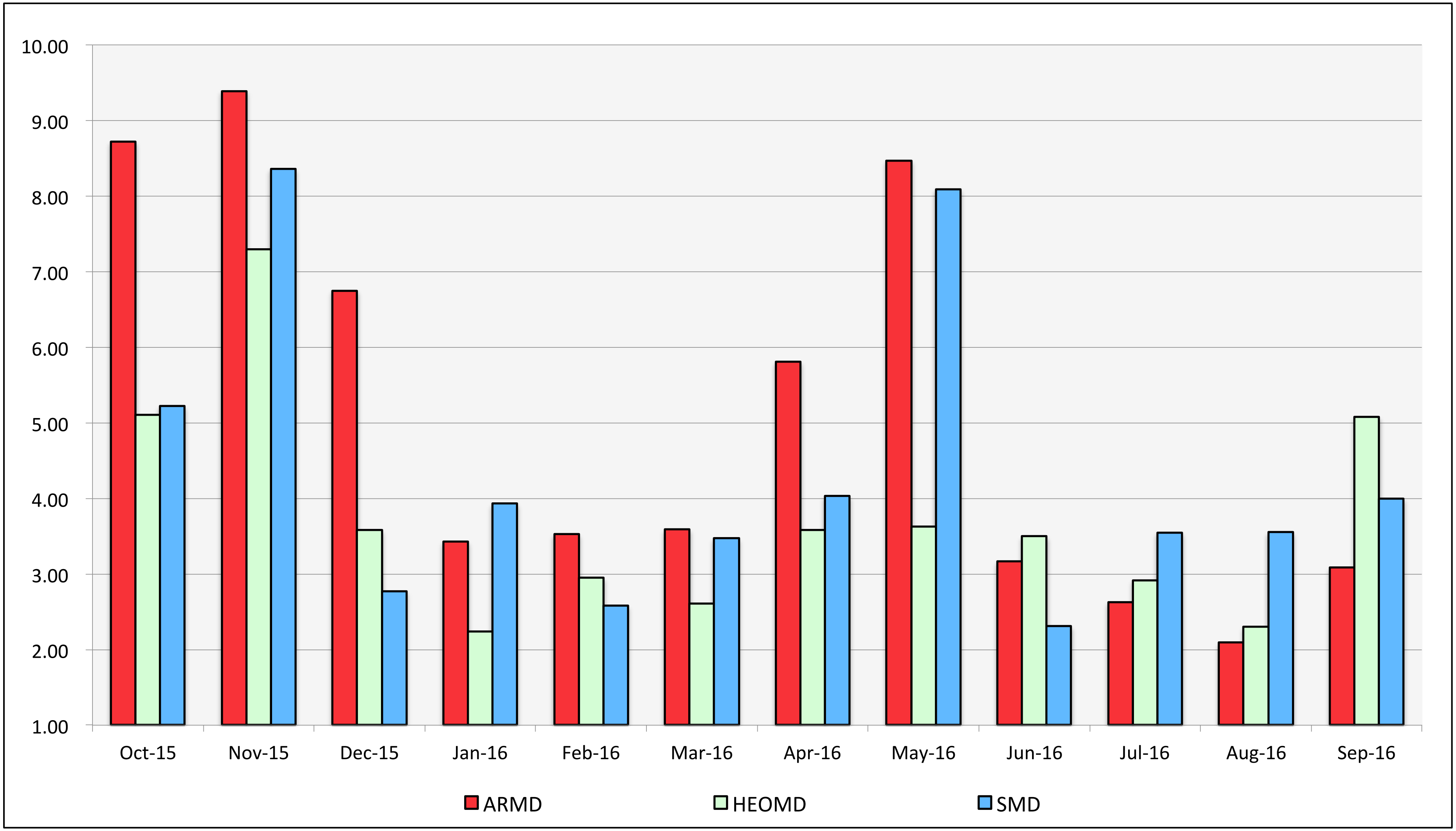
Pleiades: Monthly Utilization by Size and Length



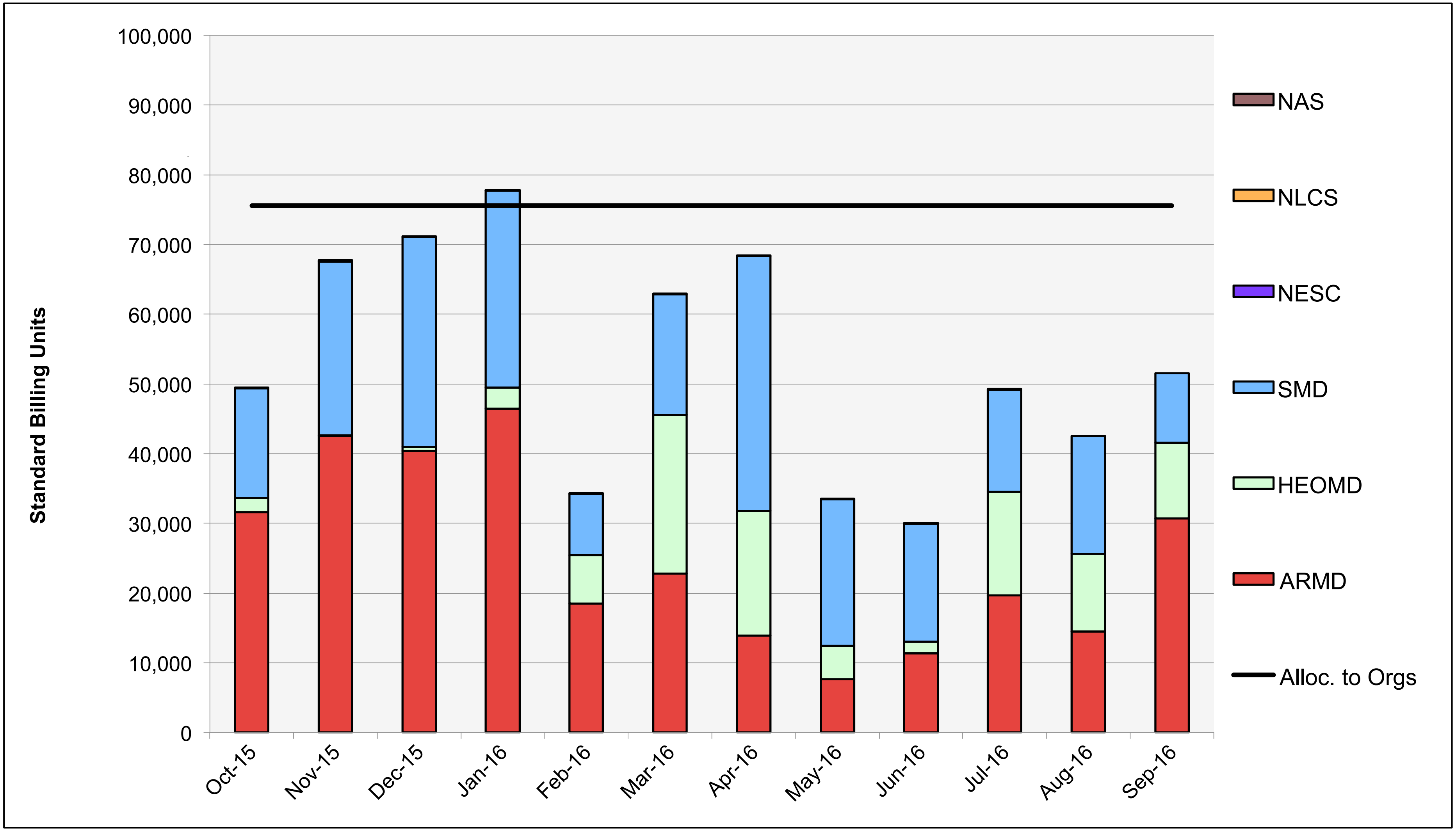
Pleiades: Average Time to Clear All Jobs



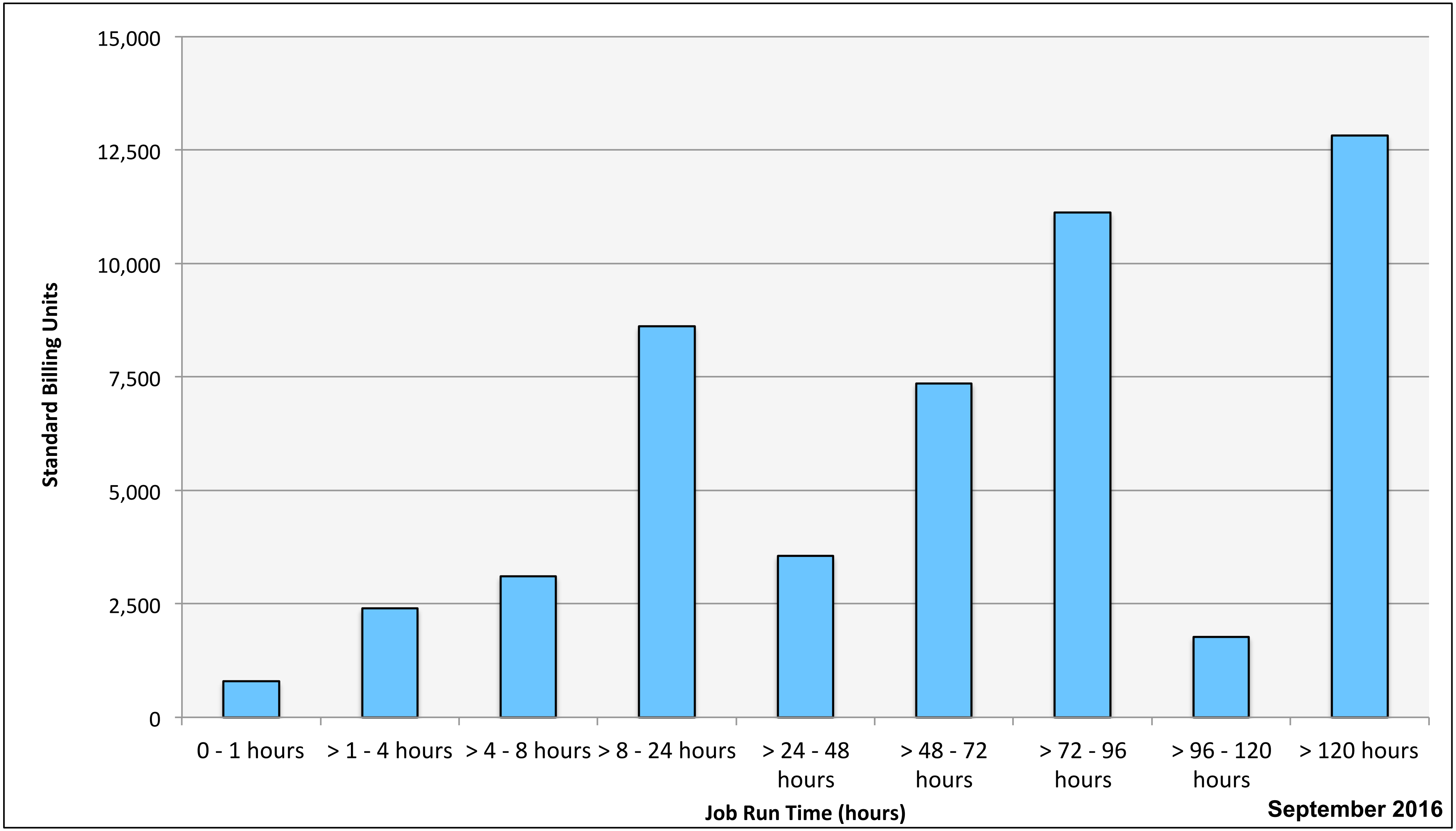
Pleiades:
Average Expansion Factor



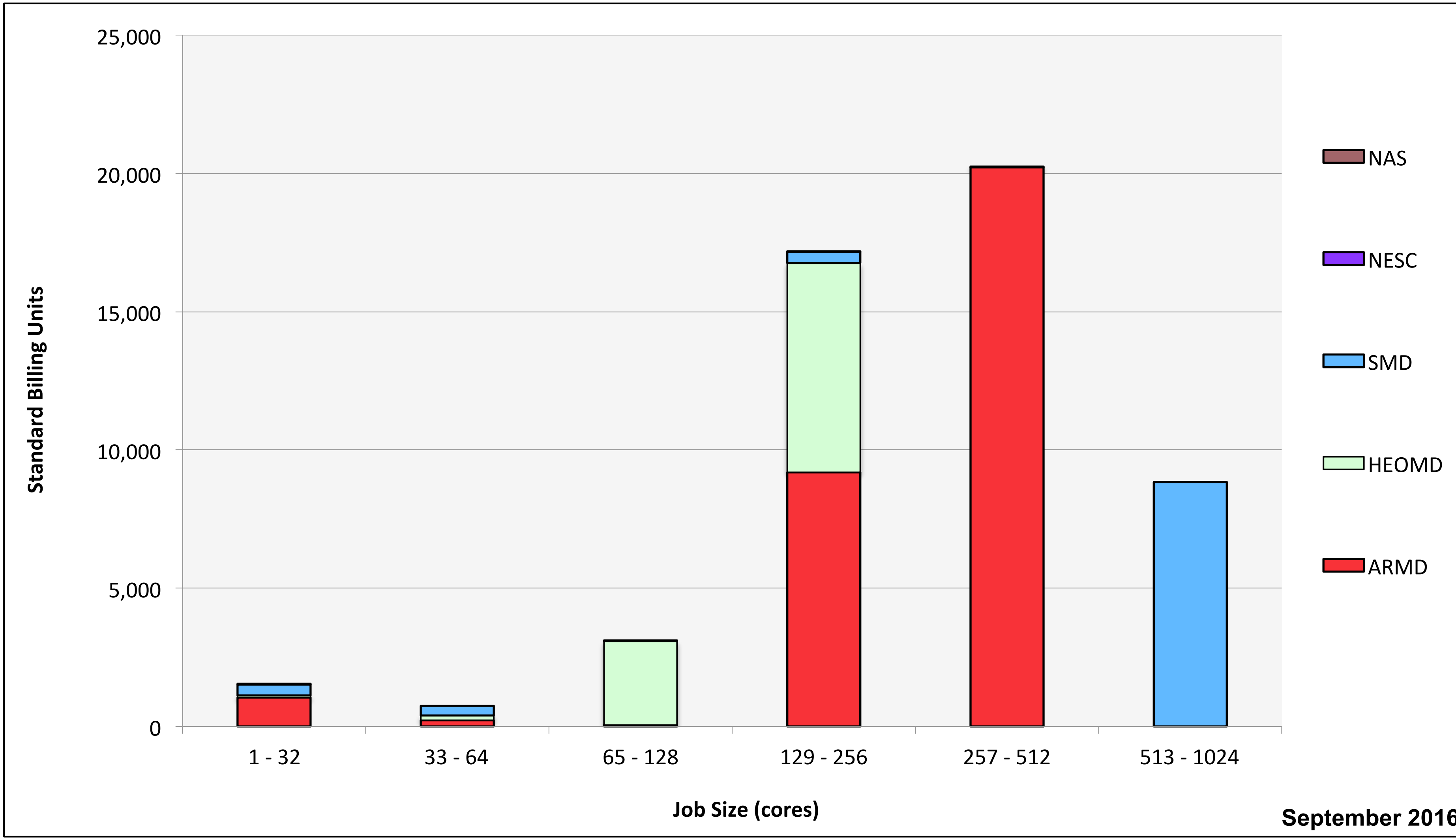
Endeavour: SBUs Reported, Normalized to 30-Day Month



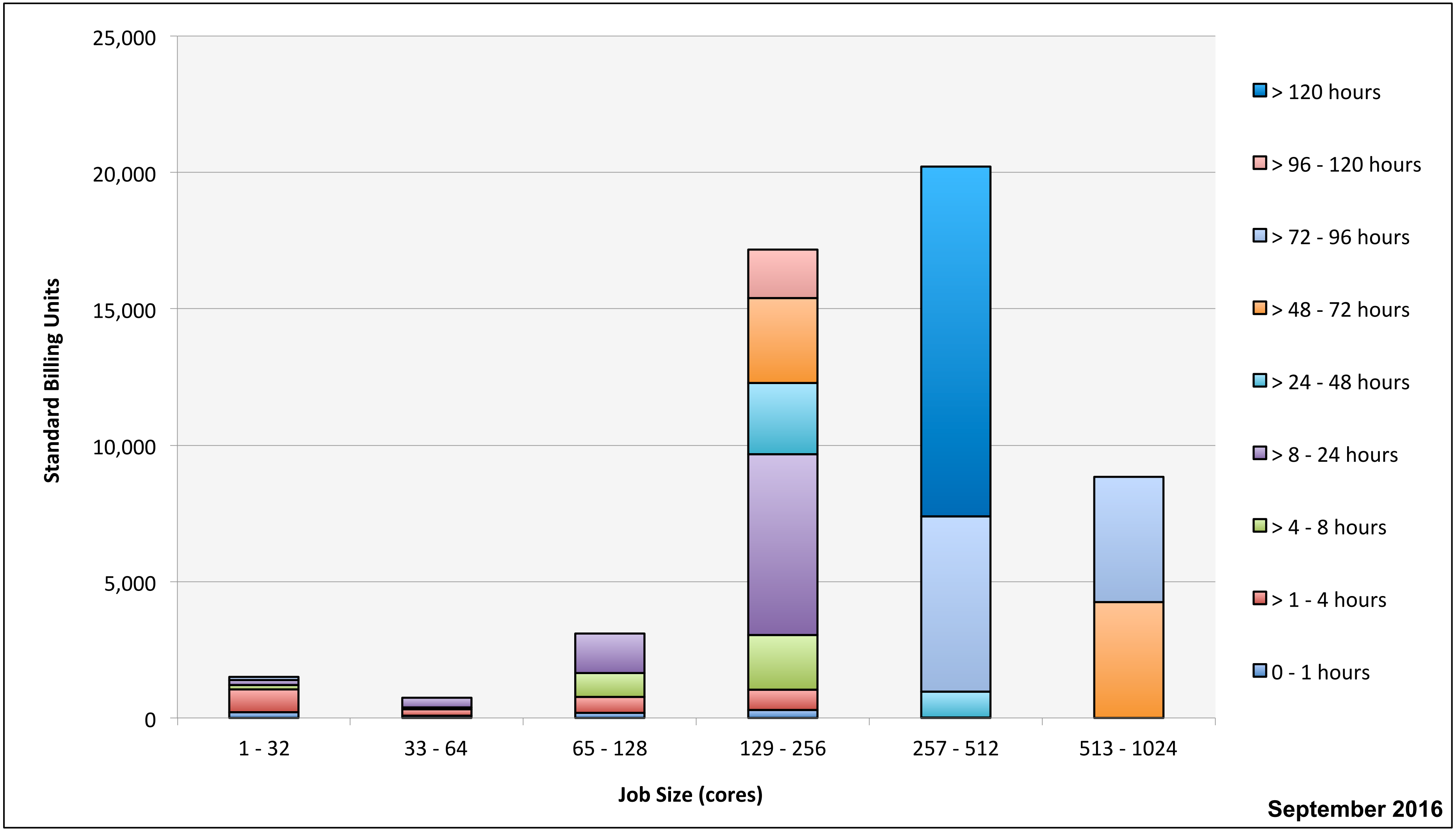
Endeavour:
Monthly Utilization by Job Length



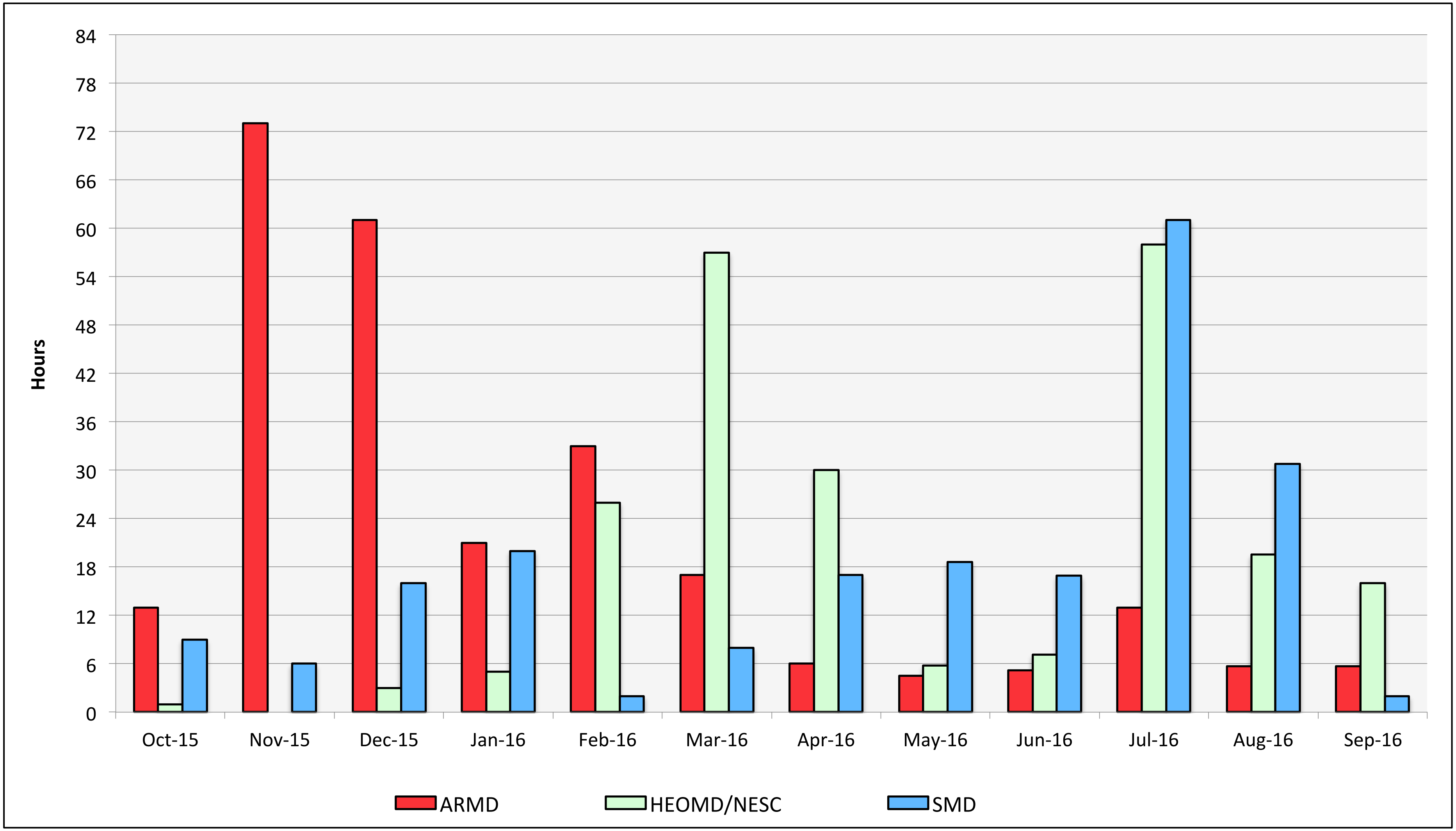
Endeavour: Monthly Utilization by Size and Mission



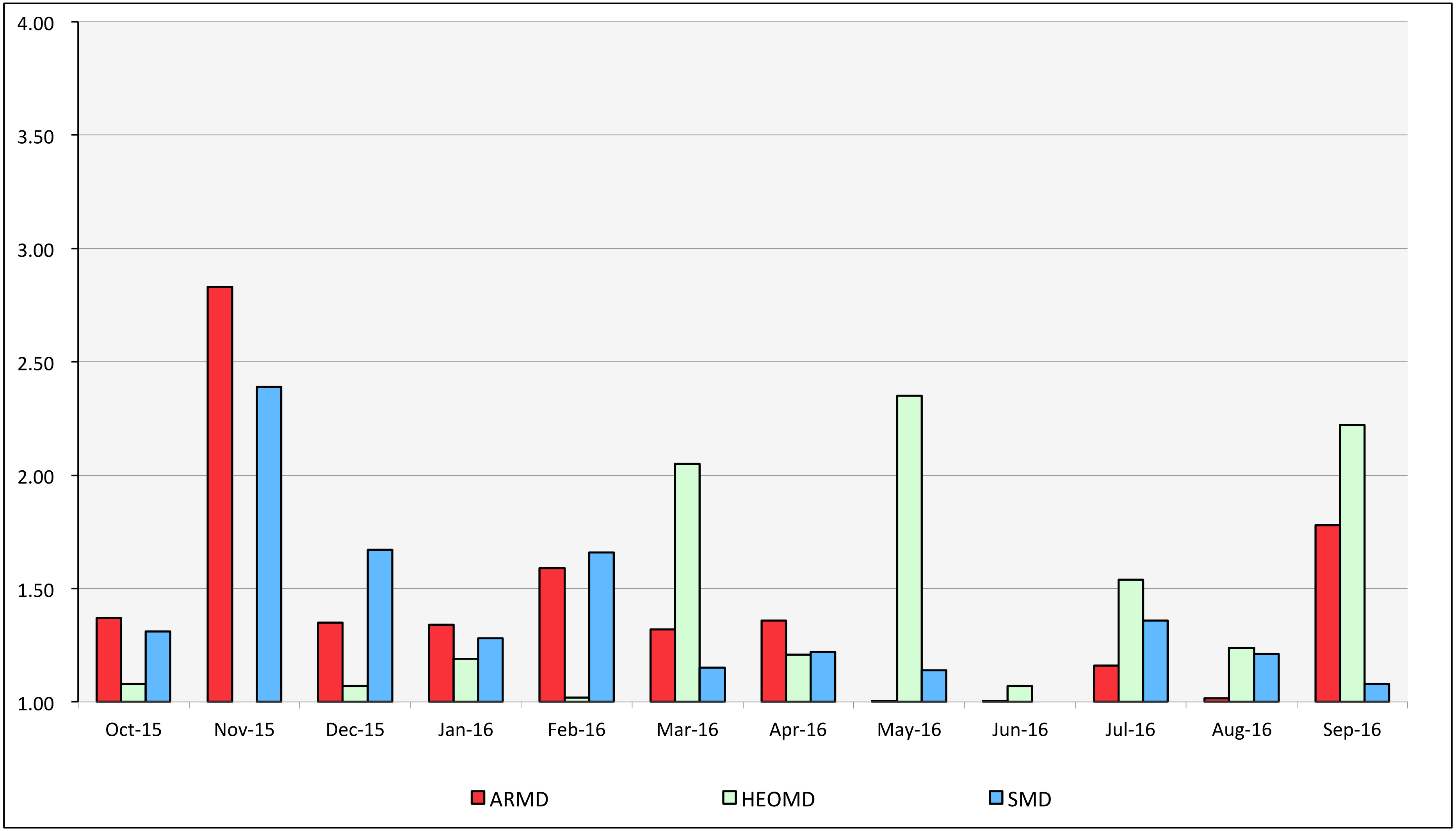
Endeavour: Monthly Utilization by Size and Length



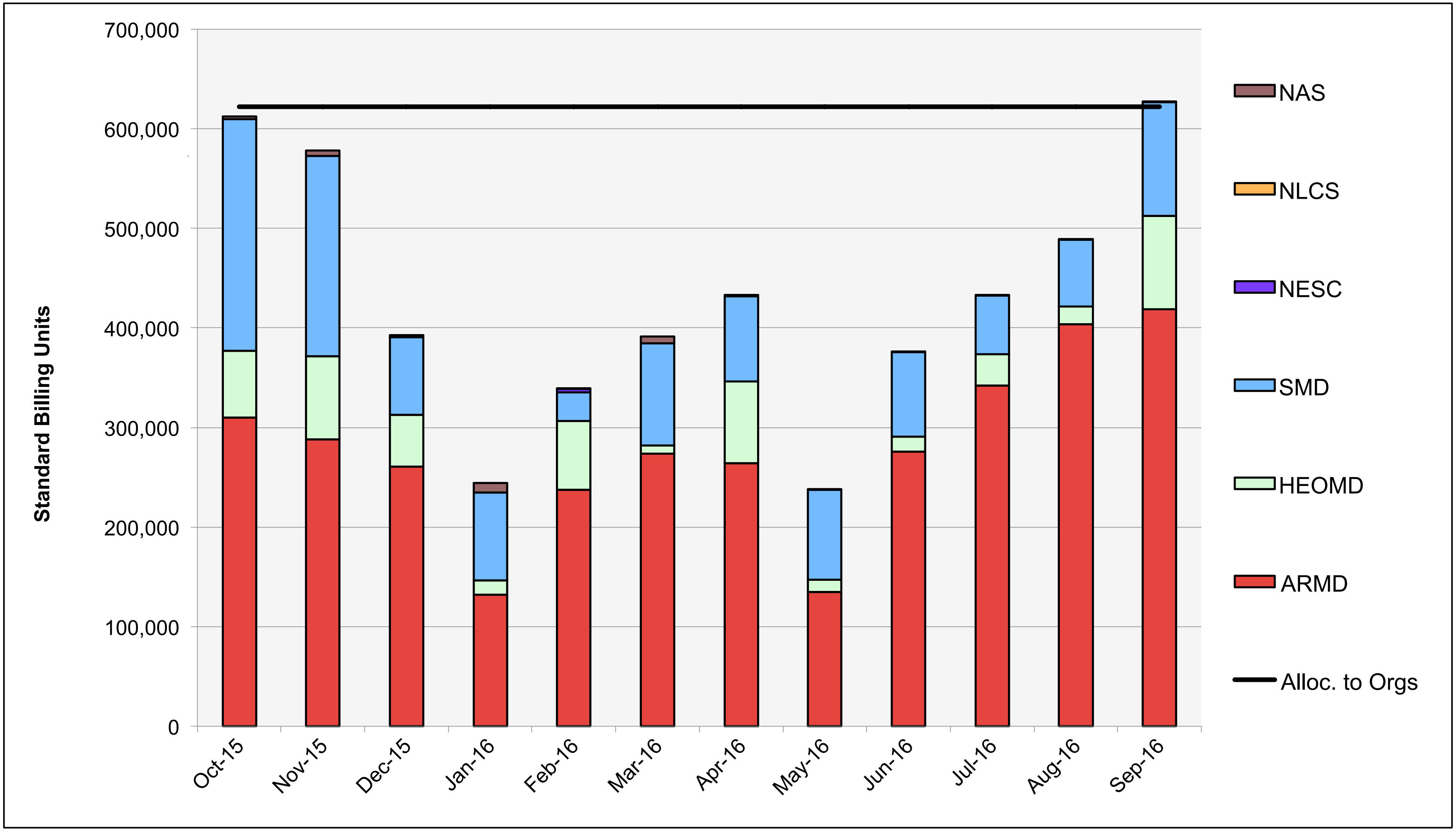
Endeavour: Average Time to Clear All Jobs



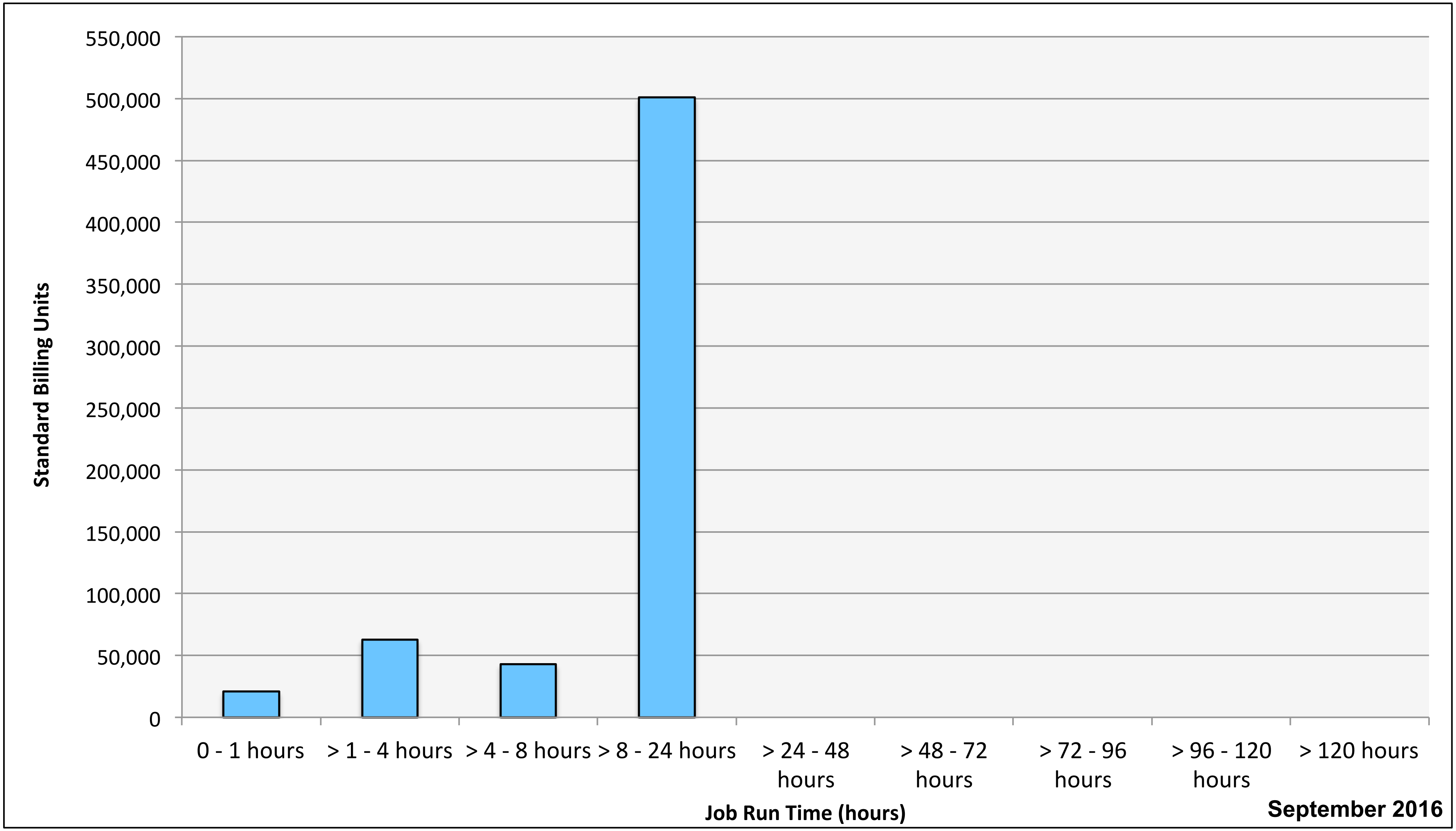
Endeavour: Average Expansion Factor



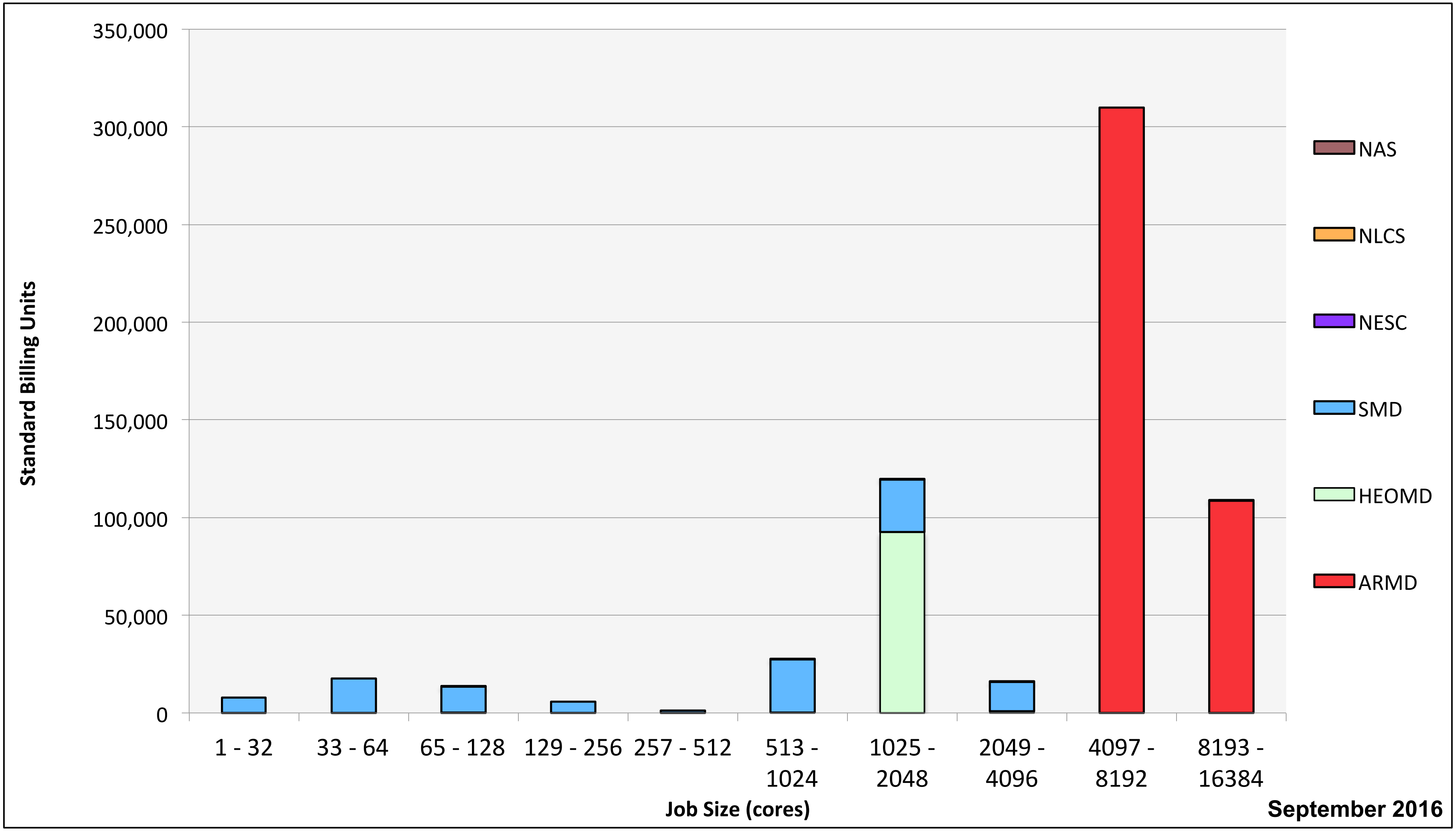
Merope: SBUs Reported, Normalized to 30-Day Month



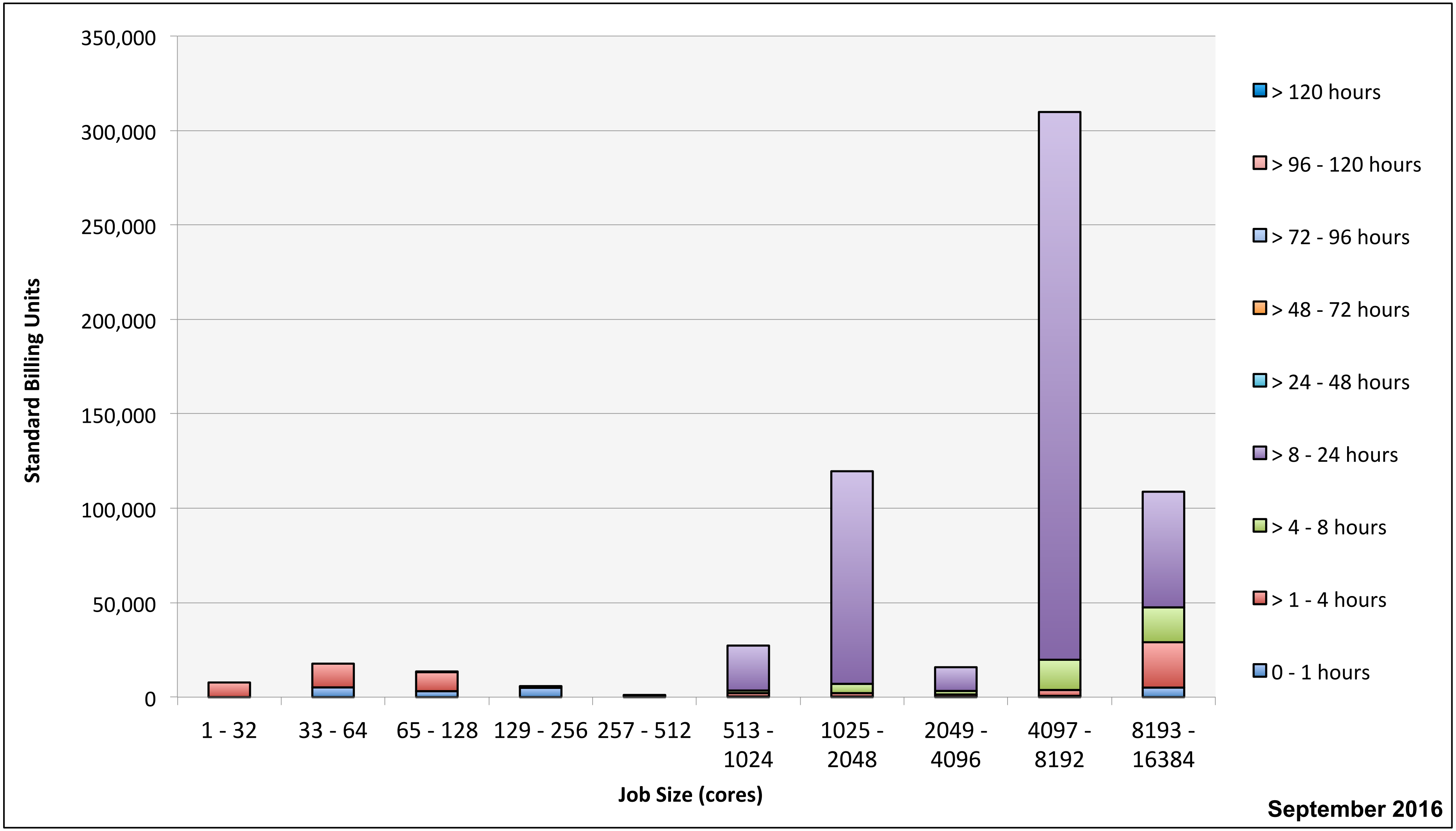
Merope:
Monthly Utilization by Job Length



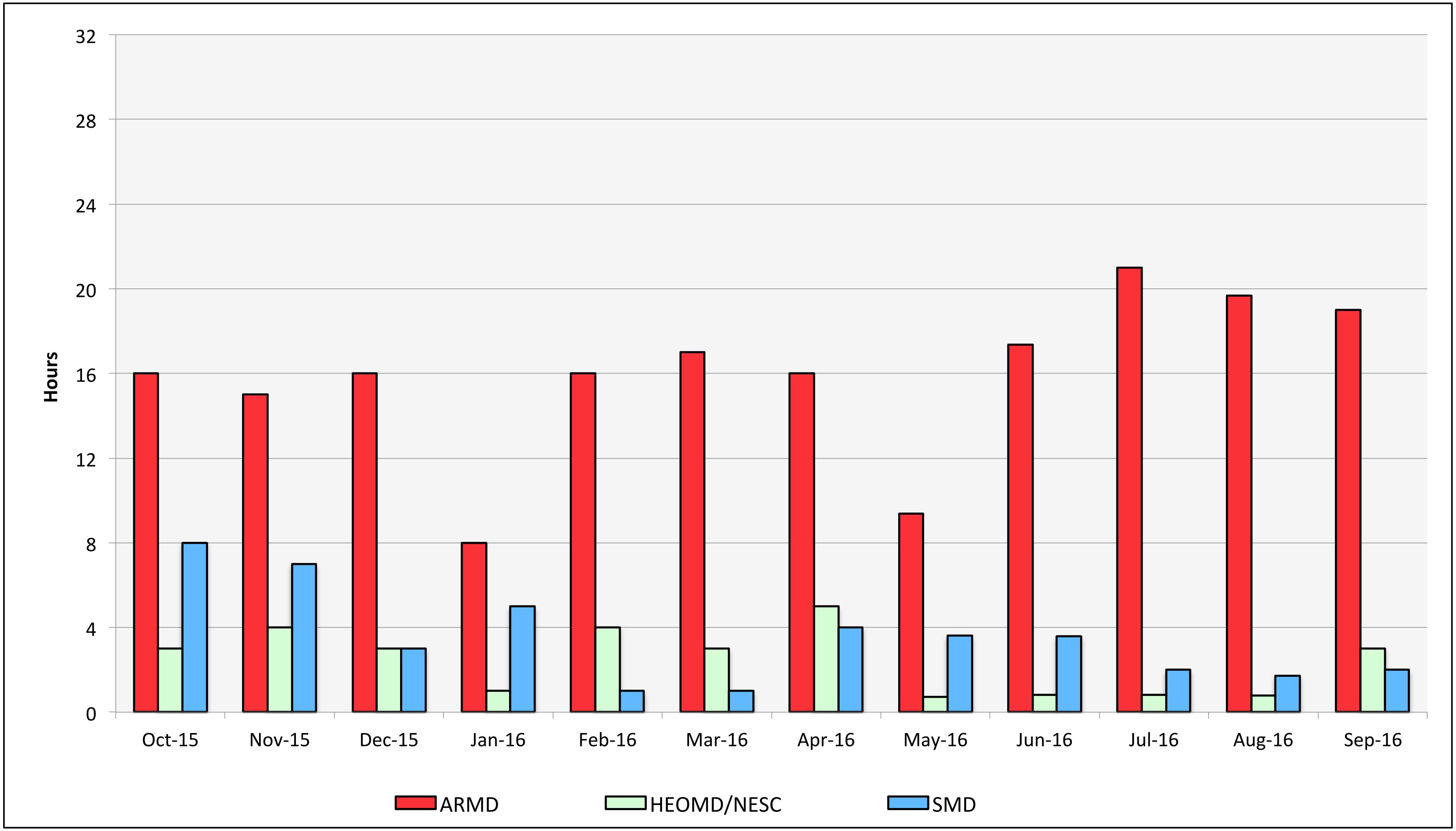
Merope:
Monthly Utilization by Size and Mission



Merope: Monthly Utilization by Size and Length



Merope:
Average Time to Clear All Jobs



Merope: Average Expansion Factor