Project Status Report

High End Computing Capability
Strategic Capabilities Assets Program

November 10, 2015

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Modular Supercomputing Facility Site Infrastructure Design Approved

- The Modular Supercomputing Facility (MSF) site infrastructure design package was approved by the NASA Ames Permit Review Board.
- HECC facilities engineers coordinated with Ames' Code J engineering and module supplier SGI/CommScope to develop site requirements and designs.
- The site was sized to accommodate two Data Center Units (DCU)-20 modules (up to 32 compute racks) and has a 2.5-megawatt power capacity to accommodate any future upgrades.
- The approved design package was provided to mechanical/electrical contractors for build-to-print bid quotations.
- Contractor selection and site construction are forecast to begin in early December and completed by March 2016.
- The initial implementation will be a proof-of-concept prototype consisting of one DCU-20 module, four compute racks, and one service rack.

Mission Impact: The MSF prototype will demonstrate the feasibility of energy-efficient modular computing, which could ultimately more than double supercomputing capability HECC provides to NASA.

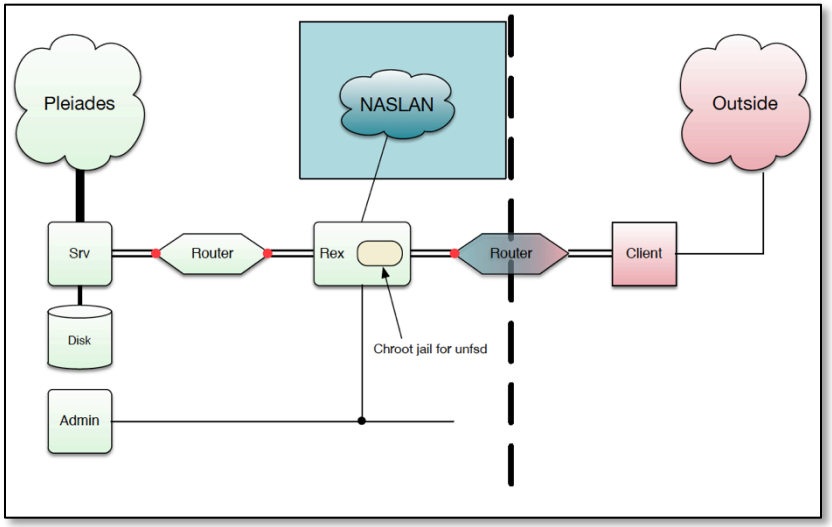
This artist's rendering of the Modular Supercomputing Facility (MSF) is shown in its actual location at NASA Ames, adjacent to the NASA Advanced Supercomputing (NAS) facility. The site is sized for two modules to be placed side by side. Utilities for the MSF will be carried to the site through underground conduits. *Marco Librero, NASA/Ames*

POCs: William Thigpen, william.w.thigpen@nasa.gov, (650) 604-1061, NASA Advanced Supercomputing (NAS) Division; Chris Buchanan, chris.buchanan@nasa.gov, (650) 604-4308, NAS Division, Computer Sciences Corp.

HECC Deploys Re-Exporter To Share Kepler Data More Efficiently

- The HECC Systems team deployed a network file system (NFS) re-exporter to share Kepler mission data more efficiently.
- The re-exporter (called keprex) enables Kepler users to easily access the data on HECC supercomputers from their remote workstations without duplicating the data.
- The Systems team first pioneered this approach for the NASA Earth Exchange (NEX) project to give users simple and secure access to the data stored within the HECC enclave via the NEX sandbox system.
- The first phase of this project enables users on remote workstations whose unique user identity information matches the keprex server information to access the Kepler data. In the second phase, keprex will enable users with different user identity information to be mapped after validation.

Mission Impact: HECC's in-house re-exporter technique enables projects to easily and securely access data stored within the HECC enclave without duplicating data.



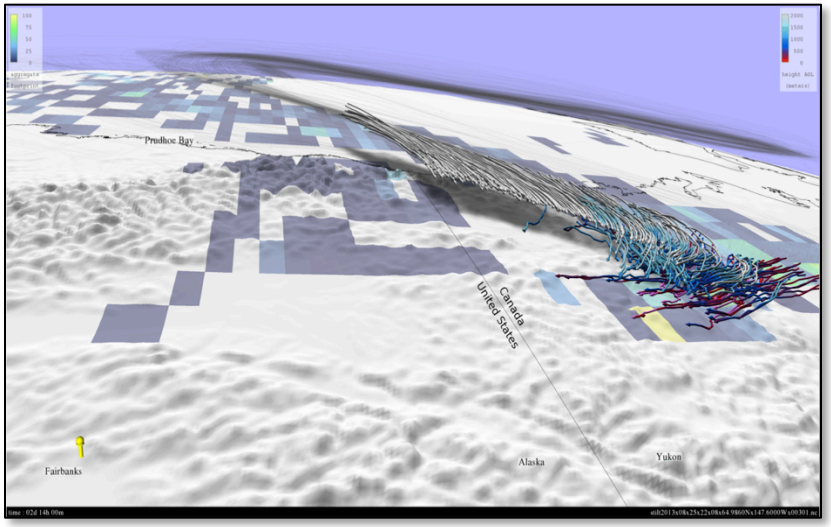
HECC's in-house Kepler re-exporter system (called keprex) accesses Kepler mission data via the InfiniBand network. Once user information is authenticated, keprex exports the data via 10 gigabit Ethernet.

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 Science Corp.

HECC Experts Modernize Job Scripts to Improve Efficiency and System Utilization

- HECC Application Performance and Productivity (APP) experts worked with John Henderson, Atmospheric and Environmental Research (AER), to improve six-year old job scripts for running the Stochastic Time-Inverted Lagrangian Transport (STILT) model, which is used for air quality studies.
- APP's new method uses a combination of GNU Parallel and PBS job arrays, which together form the most efficient and powerful way to run a battery of serial jobs.
  - In addition to greatly simplifying the job scripts, this approach keeps all other sub-jobs running when one node crashes; frees up nodes quicker to avoid idle nodes; and starts running sub-jobs on single nodes as they become available.
  - Both the GNU Parallel and PBS job arrays methods are documented in the HECC Knowledge Base.
- Henderson is "very impressed with how smoothly the runs have progressed," and will pass the new scripts to colleagues running STILT jobs at AER so that they can take advantage of this new methodology.

Mission Impact: HECC code expertise in modernizing outdated job scripts greatly simplifies workflow, and improves job turnaround time and system utilization on the Pleiades supercomputer.



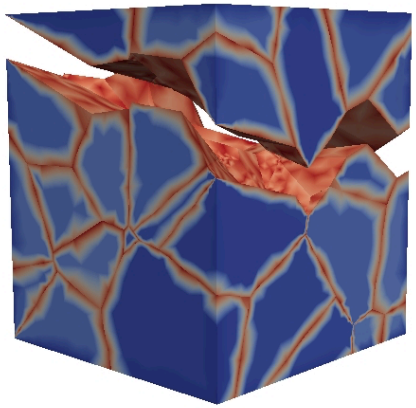
STILT tracing of 500 particles released backwards in time from the receptor location over 10 days. The image shows the last 4 hours of particle vector motion as each particle converges on the receptor location (yellow stick/ball near Fairbanks, Alaska). Particles are colored by height above ground, and turn pink when they are in the lower half of the Earth's planetary boundary layer. The cumulative footprint field, shown as the larger-scale gridded boxes on the surface, increases as the particles accumulate pollutants. *Tim Sandstrom, NASA/Ames; John Henderson, AER*

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

HECC-Langley Collaboration Doubles Performance of Aerospace Structures Code

- Continuing a long-term collaboration, HECC Application Performance and Productivity (APP) experts and an applications group at Langley Research Center (LaRC) improved performance of a code by a factor of 2.1. The teams jointly optimized the Scalable Implementation of Finite Elements by NASA (ScIFEN) code by:
  - Identifying a more efficient iterative solver and matrix preconditioner.
  - Identifying compiler flags that give the compiler more freedom to inline functions; that is, to replace a function call with a copy of the function itself.
  - Installing compiler directives to inform the compiler, freeing it to fully optimize "hot loops"—those loops where the code spends most of its time.
  - Recoding several loop nests to avoid unnecessary and expensive computation.
- ScIFEN is the third code improved through this collaboration. In each case being investigated, the teams participate in multiple WebEx sessions to review previous analysis and optimization work and brainstorm new approaches. As the LaRC staff become more comfortable with the tools and techniques, they will be better able to develop codes suitable for modern HPC systems.

Mission Impact: Doubling the performance of the ScIFEN code means researchers can simulate twice the number of fatigue cycles on an aerospace vehicle in the same amount of time. This greatly reduces reliance on lower-fidelity methods that have higher uncertainties.



The Scalable Implementation of Finite Elements by NASA (ScIFEN) code, developed with support from a NASA Aeronautics Research Institute Seedling Fund award, produces computationally demanding simulations of material behavior—such as deformation and fatigue-cracking at the micro-scale—in aerospace vehicles. This simulation image shows cracking in the microstructure of an aluminum alloy.

POCs: Dan Kokron, daniel.kokron@nasa.gov, Robert Hood, robert.hood@nasa.gov, (650) 604-0740, NASA Advanced Supercomputing (NAS) Division, Computer Sciences Corp.

ESS Team Completes Deployment of Mac OS X 10.10 to Staff Workstations

- HECC's Engineering Servers and Services (ESS) team completed the deployment of Mac OS X 10.10 (Yosemite) to 200 workstations and laptops used by staff at the NAS facility.
- The ESS team began the rollout in March, after the Security team approved the Yosemite image. Development for the Yosemite rollout included:
  - Building the NAS image using Casper.
  - Configuring security and FileVault.
  - Upgrading Casper, our Mac enterprise management tool, to the latest version.
  - Upgrading scientific software.
  - Defining the optimal upgrade process.
  - Completing a full data dump, system imaging, applications installation, encryption, and data restore for each Mac upgraded.
- Using knowledge gained from the Yosemite upgrade, ESS has already begun the download and development of the new OS X 10.11 El Capitan build.

Mission Impact: Deployment of the Mac OS X 10.10 (Yosemite) image enables HECC to support the latest Mac workstations and laptops for local scientific users and support staff.

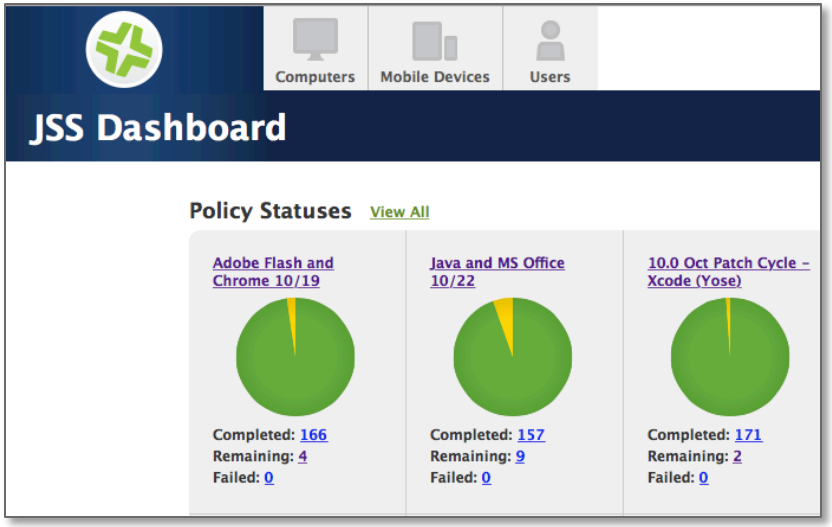
The upgrade to Mac OS X 10.10 (Yosemite) on HECC workstations and laptops is completed, and the development of the OS X 10.11 El Capitan image is now underway.

POC: Chad Tran, giang.t.tran@nasa.gov, (650) 604-2780, NASA Supercomputing Division, Computer Sciences Corp.

Casper Server Now Accessible Over NAS VPN to Improve Mac Patching

- To improve the process of patching Macs to ensure that critical patches are applied as efficiently as possible, the HECC Networks and Engineering Servers and Services (ESS) teams opened up the Casper enterprise management server to the NAS virtual private network (VPN).
- Previously, the Casper server was only reachable by systems on the local NAS Ethernet. To allow patching of Macs on the NAS VPN, HECC staff took the following actions:
  - Obtained security review and approval of proposed service configuration.
  - Opened up necessary ports to allow the Casper server to be accessible on the VPN.
  - Modified Casper to recognize Mac addresses of systems on the VPN, rather than recognizing only IP addresses.
- Security patches and monthly update patches can now be easily applied to systems used by HECC/ NAS staff who are on travel, on leave, at remote locations, or telecommuting.

Mission Impact: By improving the process of applying security patches to staff systems not connected to the local network, HECC system administrators increase their ability to manage patches and reduce the risk of successful attacks on user systems.



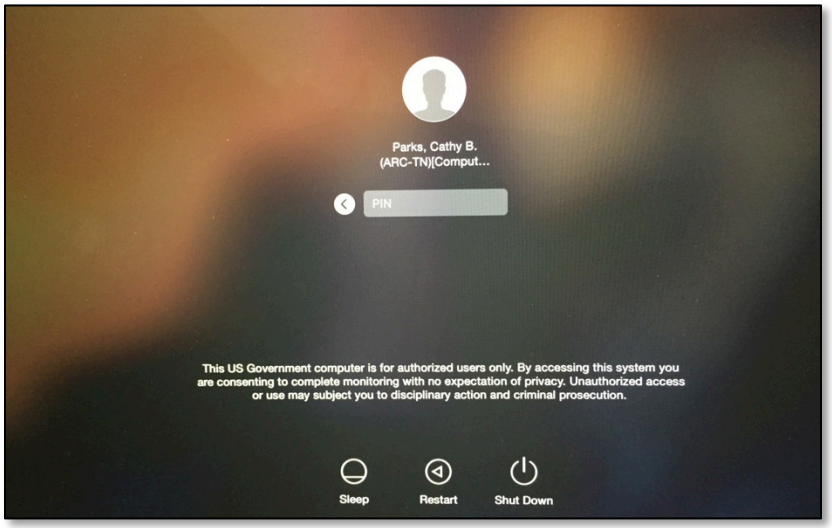
The Casper application is now accessible on the NAS virtual private network to quickly push out the increasing number of Macintosh security patches.

POCs: Chris Shaw, robert.c.shaw@nasa.gov, (650) 604-4354, Harjot Sidhu, harjot.s.sidhu@nasa.gov, (650) 604-4935, NASA Supercomputing Division, Computer Sciences Corp.

ESS Team Rolls Out Beta Test of PIV Authentication on the Mac Using Centrify

- To meet NASA's new requirement for multi-factor authentication on user systems, HECC's Engineering Servers and Services (ESS) team rolled out a Mac beta test of Personal Identity Verification (PIV) smartcard authentication using the Centrify software.
- ESS worked through numerous issues to achieve the successful beta deployment, including:
  - Obtained a NASA Data Center (NDC) organizational unit and Centrify Zone technology, defined for our systems to allow ESS to manage the systems with the Centrify Server Suite.
  - Developed and managed an account to authenticate to FileVault and bring up the login window for PIV authentication.
  - Developed machine-based enrollment through configuration files for PIV authentication that will not lock out legacy technologies (such as wireless) that cannot use PIV authentication.
- Full rollout of Mac PIV smartcard authentication to staff is expected to start in early November.

Mission Impact: Transitioning HECC Mac systems to use PIV smartcards for computer login meets government-wide access requirements and will provide NASA with a proven model to role out to all NASA Mac users.



Once the smartcard authentication method is in place on Macs at the NASA Advanced Supercomputing facility, staff will be prompted for a smartcard PIN instead of an NDC password to complete authentication to their systems.

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

Developing Computational Aeroacoustics Tools for Airframe Noise Prediction *

- Computational aeroacoustics (CAA) plays a critical role in understanding and characterizing noise-generation sources for aircraft component designs. Modeling and simulation experts at NASA Ames are developing state-of-the-art CAA tools and predictive capabilities with their Launch Ascent and Vehicle Aerodynamics (LAVA) code.
- Using LAVA to run parallel computations across thousands of Pleiades nodes, the researchers:
  - Demonstrated and validated high-fidelity, time-accurate, higher-order computational methods for complex noise-prediction problems.
  - Utilized far-field noise propagation techniques to identify major airframe noise frequencies and sources.
  - Assessed two analytical benchmark problems to advance techniques for predicting noise generated by landing gear and by the leading-edge slat of a high-lift wing—major contributors to aircraft noise during landing.
  - Improved the resolution of unsteady flow features in simulations of the Four Jet Impingement Device, which is used to experimentally reproduce the broadband noise signatures of aircraft engines.
- Results compare well with experimental and computational results for key benchmark problems, and the innovative techniques provide an excellent method for future simulations.

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

Mission Impact: Reducing aircraft noise is a goal of NASA's Aeronautics Research Mission Directorate. With the help of computational aeroacoustics tools and predictive capabilities, next-generation aircraft can meet more stringent noise-generation standards.

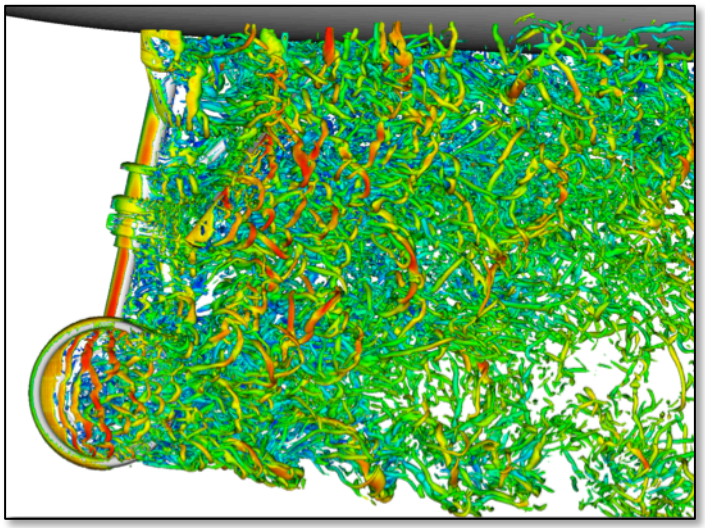
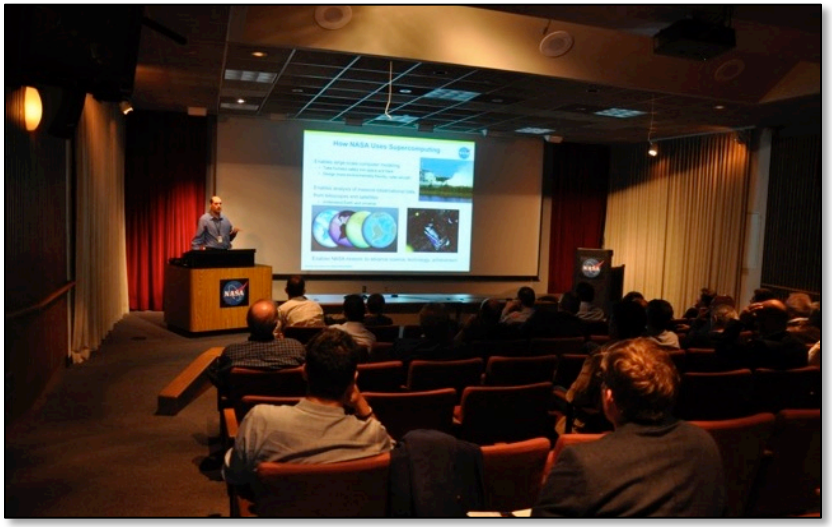


Image from a computational aeroacoustics simulation of landing gear for a benchmark airframe noise problem. The flow field is shown with isocontours of the q-criterion (a measure of vorticity) colored by Mach number. The simulation was computed on the Pleiades supercomputer using the Launch Ascent and Vehicle Aerodynamics (LAVA) code. *Michael Barad, NASA/Ames*

POCs: Cetin Kiris, cetin.c.kiris@nasa.gov, (650) 604-4485, NASA Advanced Supercomputing Division.

HECC Facility Hosts Several Visitors and Tours in October 2015

- HECC hosted 7 tour groups in October. Guests learned about the agency-wide missions being supported by HECC assets; some groups also viewed the expanded D-Wave quantum computer system. Visitors this month included:
  - Veronica La Regina, a former International Space University professor and current senior researcher for the Italian Space Agency, who was a guest of ARC management.
  - 18 ARC fall interns, as part of an Ames center tour.
  - 50 attendees of the International Forum for Aviation Research (IFAR) Summit 2016 toured the facility; this annual meeting was held at ARC, and the group included representatives from 25 countries.
  - The National Space Society received tours of various ARC facilities, including HECC.
  - 45 executives from major Spanish companies, who visited Silicon Valley as part of an Innovation Tour organized by Oracle. (The organizer requested a visit to ARC as part of the agenda.) Attendees included chief information officers, chief technology officers, and chief innovation officers.
  - 40 French business executives from Rebellion Labs toured ARC to learn about how NASA conducts public/ private partnerships and transfers technology from the public to private sector.



Bryan Biegel, NAS deputy division chief, presented an overview of HECC project capabilities and services to Rebellion Lab guests, and gave them a tour of the Pleiades supercomputer room.

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

Papers

- "**HEROIC: 3D General Relativistic Radiative Postprocessor with Comptonization for Black Hole Accretion Disks**," R. Narayan, Y. Zhu, D. Psaltis, A. Sadowski, arXiv: 1510.04208 [astro-ph.HE], October 14, 2015. * *http://arxiv.org/abs/1510.04208*
- "**Compressibility and Density Fluctuations in Molecular-Cloud Turbulence**," L. Pan, P. Padoan, T. Haugbolle, A. Nordlund, arXiv:1510.04742 [astro-ph.GA], October 15, 2015. * *http://arxiv.org/abs/1510.04742*
- "**Formation of Globular Clusters in Atomic-Cooling Halos via Rapid Gas Condensation and Fragmentation During the Epoch of Reionization**," T. Kimm, R. Cen, J. Rosdahl, S. Yi, arXiv:1510.05671 [astro-ph.GA], October 19, 2015. * *http://arxiv.org/abs/1510.05671*
- "**Structure in Galaxy Distribution. III. Fourier Transforming the Universe**," J. Scargle, M. Way, P. Gazis, arXiv:1510.06129 [astro-ph.CO], October 21, 2015. * *http://arxiv.org/abs/1510.06129*

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

Presentations

- "**Implementation of an Open-Scenario, Long-Term Space Debris Simulation Approach**," J. Stupl, B. Nelson, presented at the Advanced Maui Optical and Space Surveillance Technologies Conference (AMOS), Maui, HI, September 20–23, 2015.*
- "**Hybrid Electric Distributed Propulsion Technologies for Large Commercial Aircraft: A NASA Perspective**," N. Madavan, presented at the 2015 IEEE Energy Conversion Congress & Exposition, Montreal, Canada, September 21–24, 2015.*
- "**Evaluating and Improving HECC User Project Productivity**," W. Thigpen, presented at the HECC Board of Advisors Meeting in Washington D.C., October 22, 2015.

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

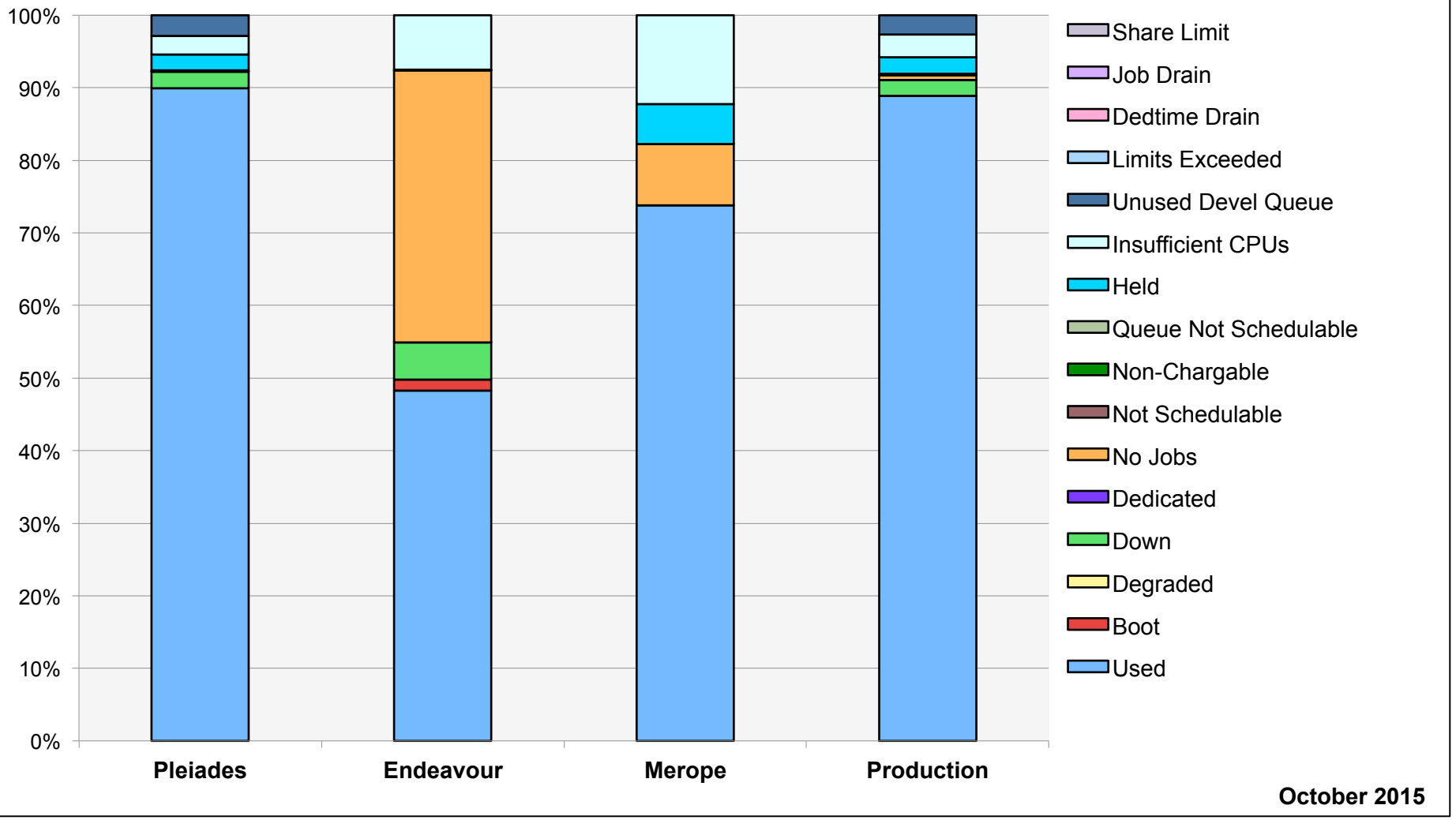
News and Events

- **Explosions and Plasma Jets Associated with Sunspot Formation Revealed**, *Space Daily*, October 5, 2015—A team of scientists analyzed observations of sunspots from the Solar Dynamics Observatory (SDO) and the Interface Region Imaging Spectrograph (IRIS) missions by performing numerical simulations on the Pleiades supercomputer.
  http://www.spacedaily.com/reports/Mechanism_of_explosions_and_plasma_jets_associated_with_sunspot_formation_revealed_999.html
- **Video: Prologue O/S—Improving the Odds of Job Success**, *insideHPC*, October 12, 2015—In this video from the 2015 PBS Works User Group meeting, Dale Talcott from the NASA Advanced Supercomputing (NAS) Division discusses how NAS has customized PBS to identify problem nodes before running jobs.
  http://insidehpc.com/2015/10/video-prologue-os-improving-the-odds-of-job-success/
- **SC15 Releases Short Video Explaining Why High Performance Computing is Important to NASA**, *The Official SC15 Blog,* October 15, 2015—In this video, NAS Division aerospace engineer Shishir Pandya explains how HPC helps advance airplane and rocket technologies to save fuel and make travel more affordable for the public.
- **How HPC is Helping Define the Future of Aviation**, *Scientific Computing*, October 20, 2015—As a follow up to the SC15 #HPCMatters video, Shishir Pandya blogs about how NASA uses supercomputers to help design fuel-efficient aircraft.
  http://www.scientificcomputing.com/blogs/2015/10/how-hpc-helping-define-future-aviation

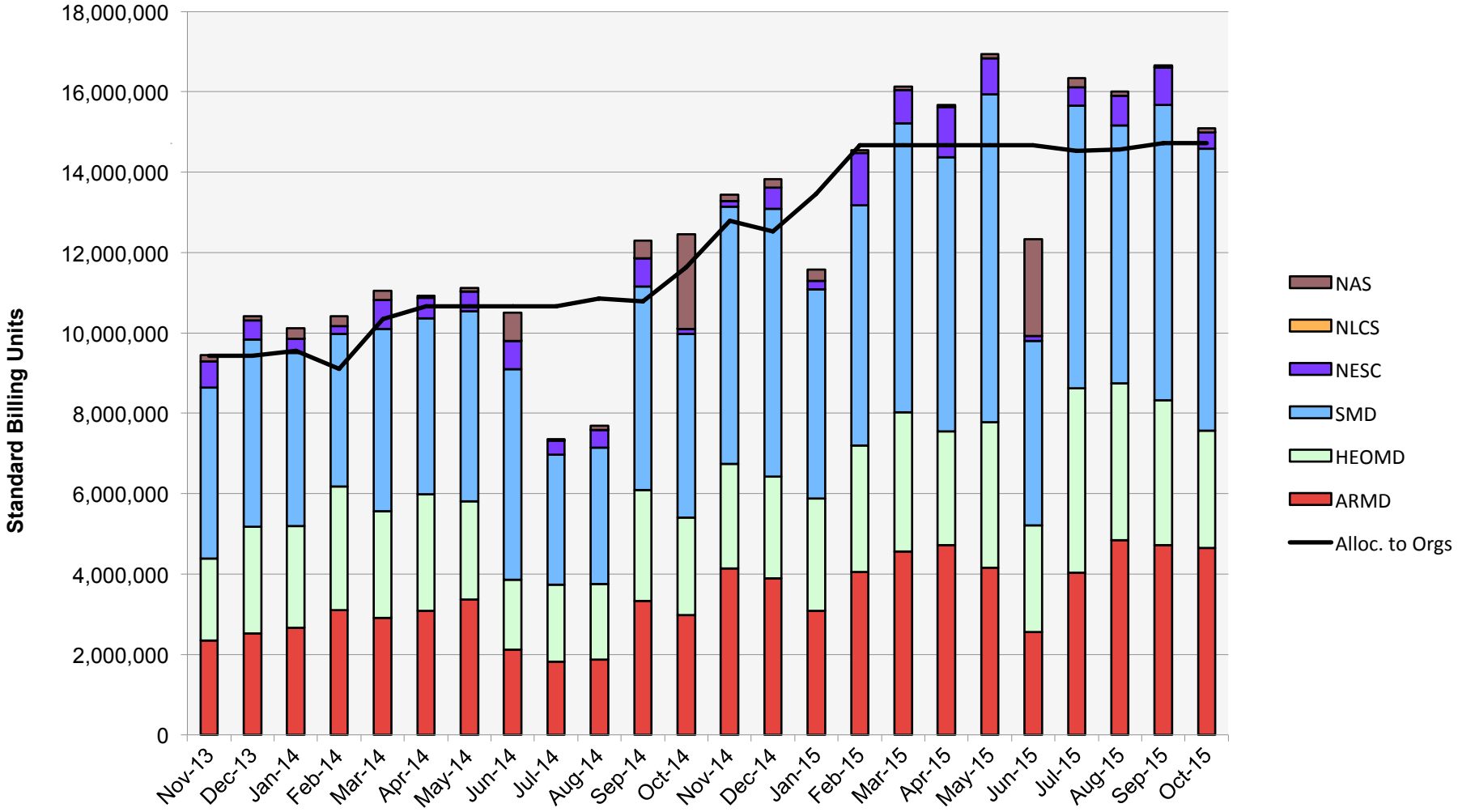
News and Events

- **Central Valley Idle Farmland Doubling During Drought**, *Central Valley Business Times,* October 26, 2015—The current drought has idled more than 1.03 million acres of land in the Central Valley, roughly 15 percent of the 7 million acres of irrigated farmland in the Valley, according to a study by NASA, in collaboration with the USDA, USGS, and the California Department of Water Resources. The compute-intensive analysis was conducted through the NASA Earth Exchange using HECC resources at the NAS facility.
  http://www.centralvalleybusinesstimes.com/stories/001/?ID=29314
  - **Idle Farmland In California's Central Valley Doubles During Drought**, Growing Produce, October 27, 2015.
    http://www.growingproduce.com/vegetables/idle-farmland-in-californias-central-valley-doubles-during-drought/
- **SGI Reports Fiscal First Quarter 2016 Financial Results**, *SGI press release*, October 28, 2015—SGI releases their first quarter financial results for 2016, highlighting recent achievements, including Pleiades' debut at number five on the June 2015 HPCG benchmark list.
  http://investors.sgi.com/releasedetail.cfm?ReleaseID=939024
  - **SGI Reports Fiscal First Quarter 2016 Financial Results**, *HPCwire*, October 29, 2015.
    http://www.hpcwire.com/off-the-wire/sgi-reports-fiscal-first-quarter-2016-financial-results/

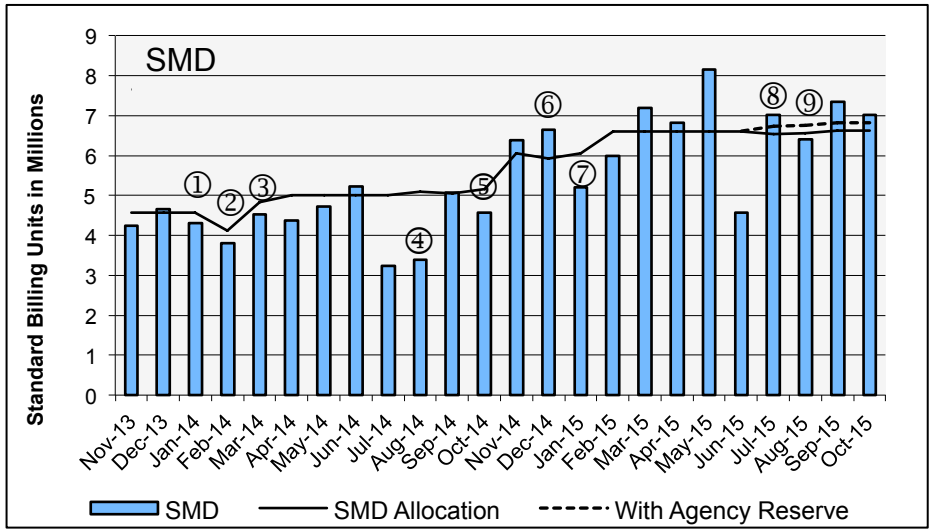
HECC Utilization

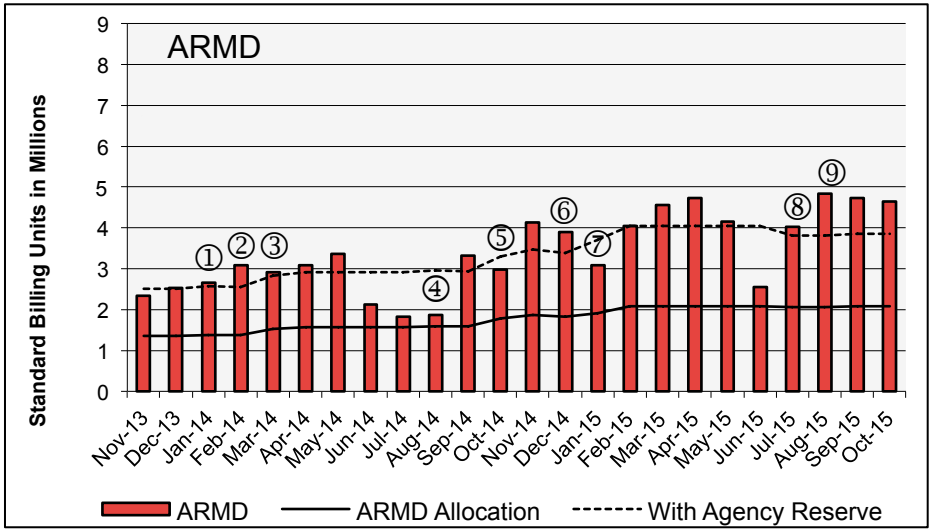


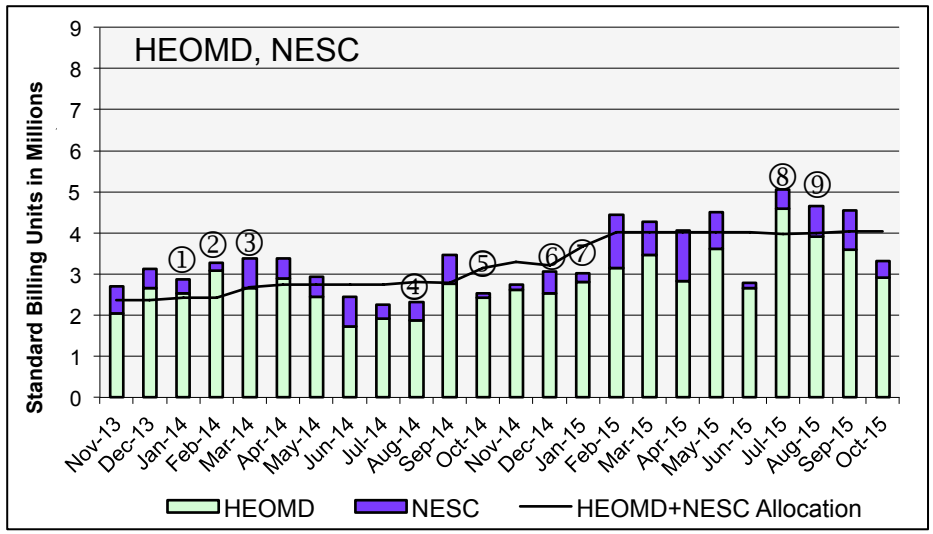
HECC Utilization Normalized to 30-Day Month



HECC Utilization Normalized to 30-Day Month







① 6 Ivy Bridge Racks added; 20 Nehalem, 12 Westmere Racks Retired from Pleiades

② 8 Ivy Bridge Racks added mid-Feb; 8 Ivy Bridge Racks added late Feb to Pleiades

③ 4 Ivy Bridge Racks added mid-March to Pleaides

④ 6 Westmere Racks added to Merope, Merope Harpertown retired

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

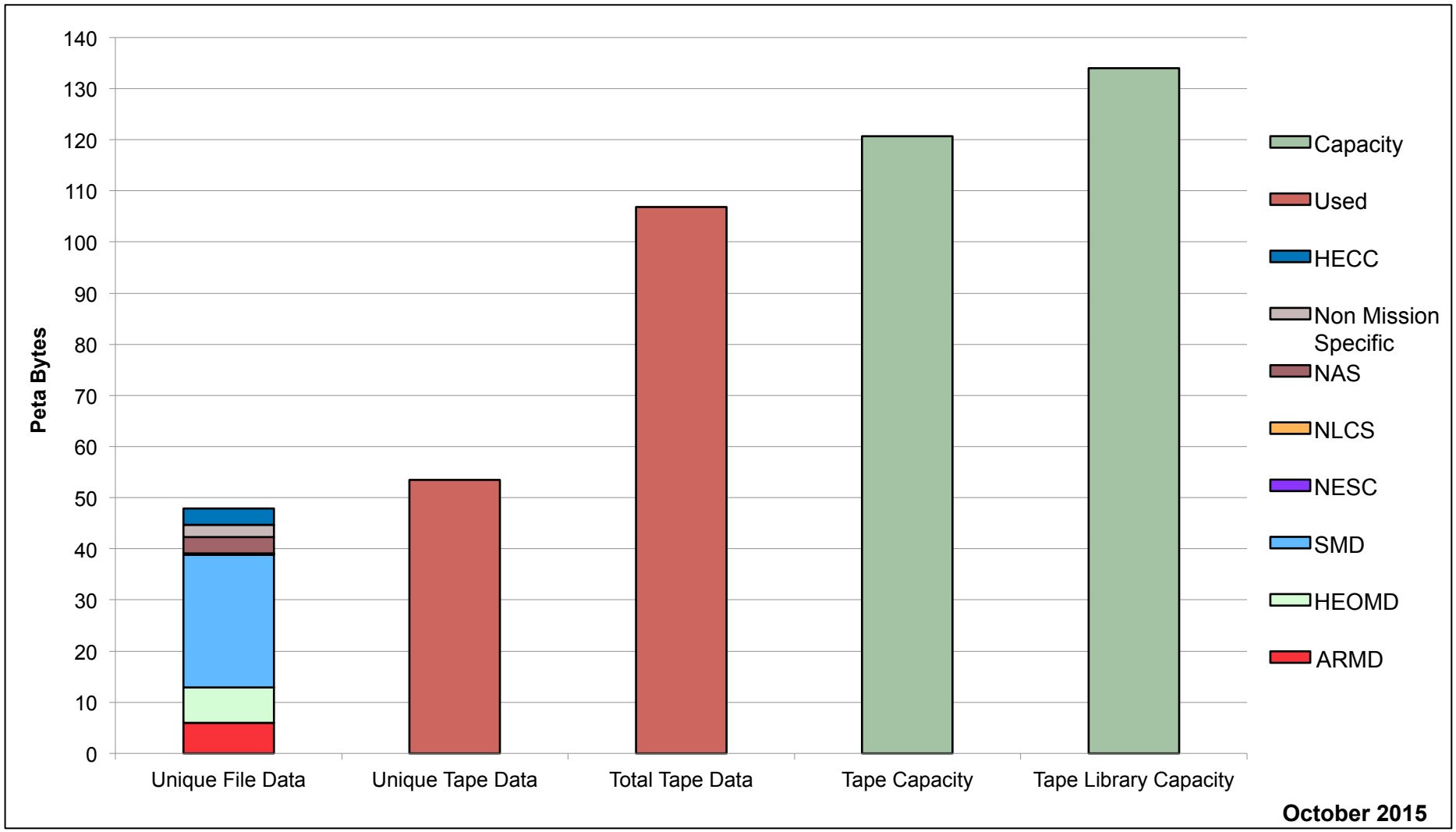
⑥ 16 Westmere Racks retired from Pleiades

⑦ 14 Haswell racks added to Pleiades

⑧ 7 Merope Nehalem Racks removed from Merope

⑨ 7 Merope Westmere Racks added from Merope

Tape Archive Status



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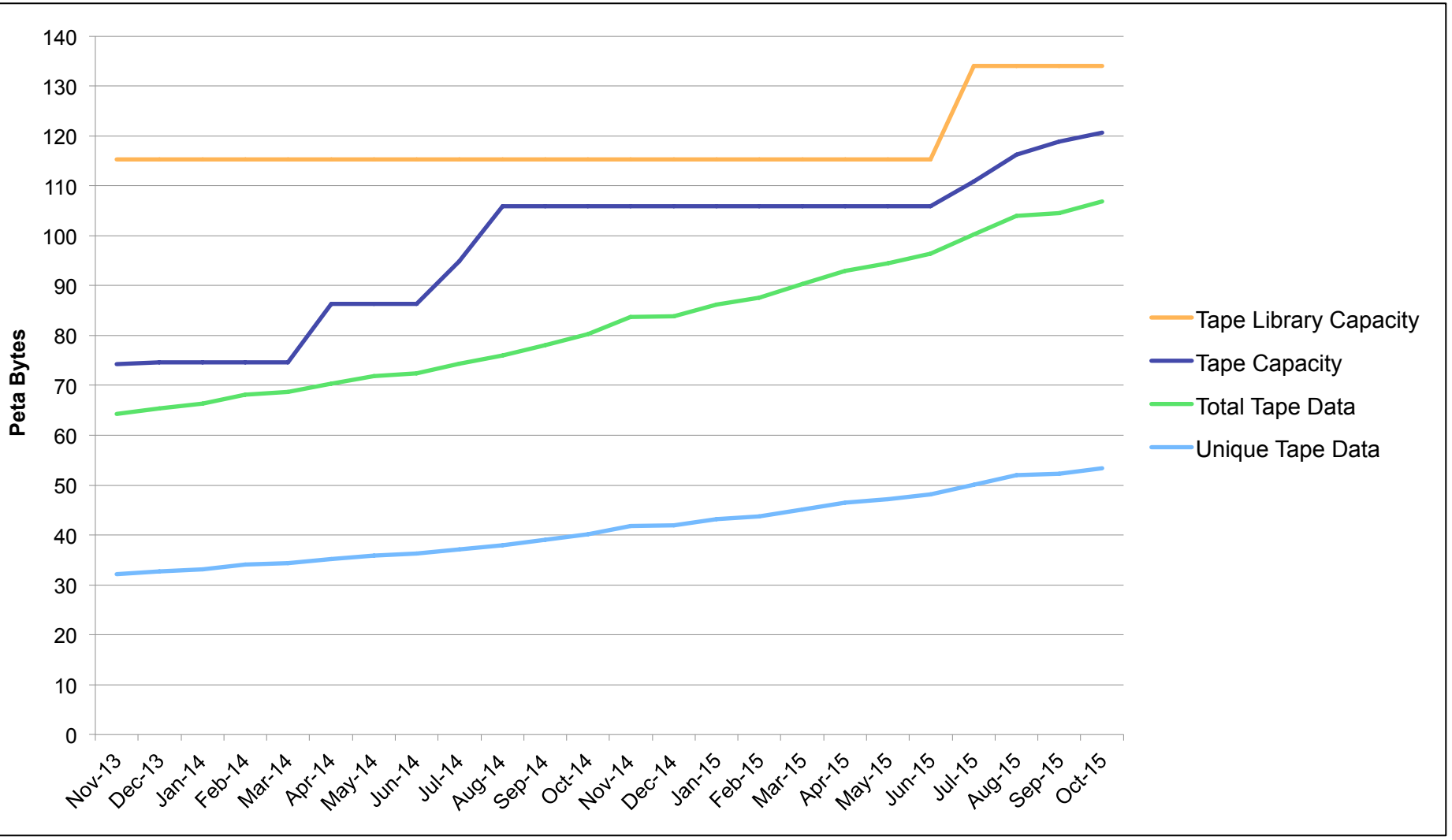
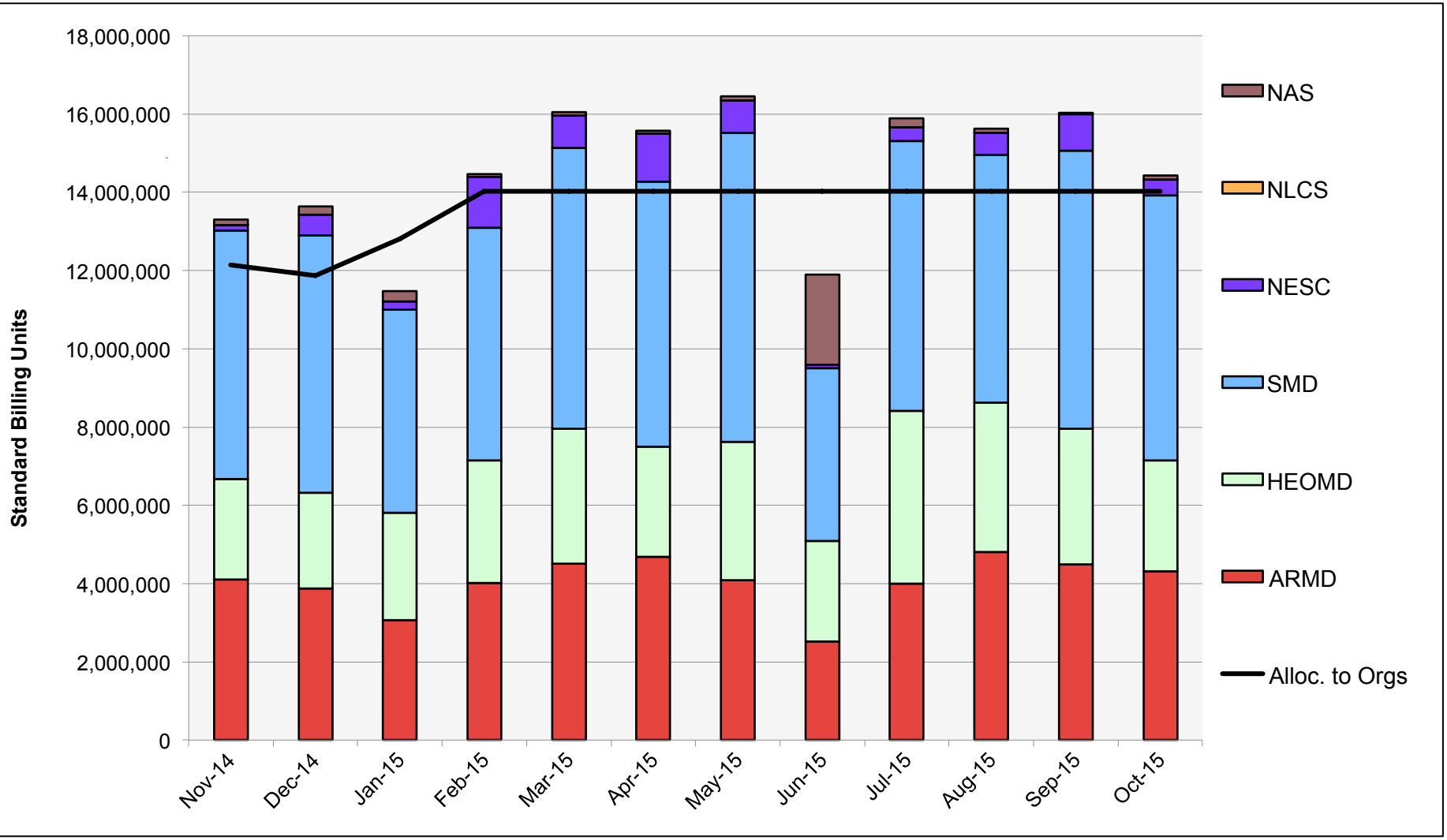
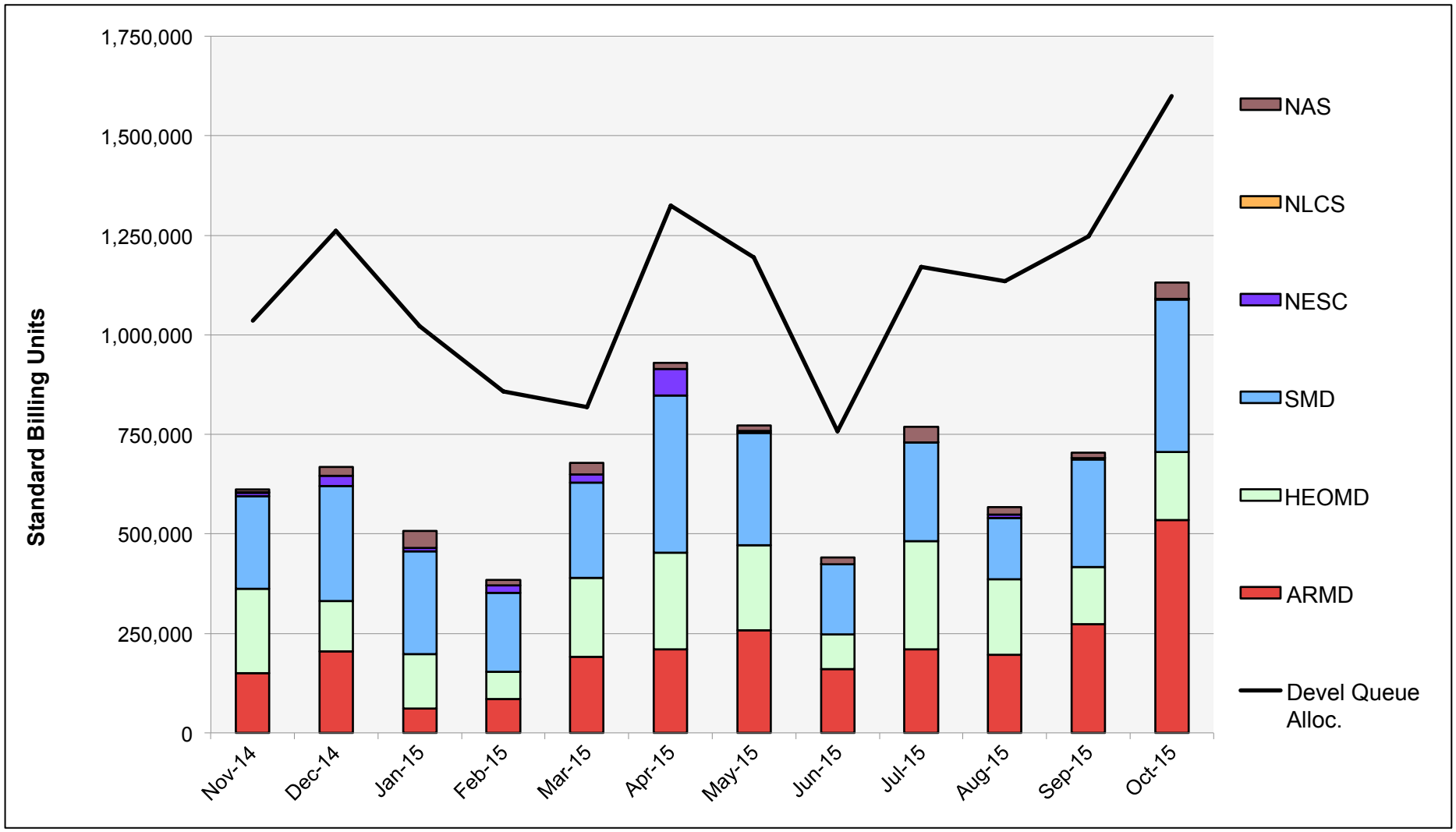


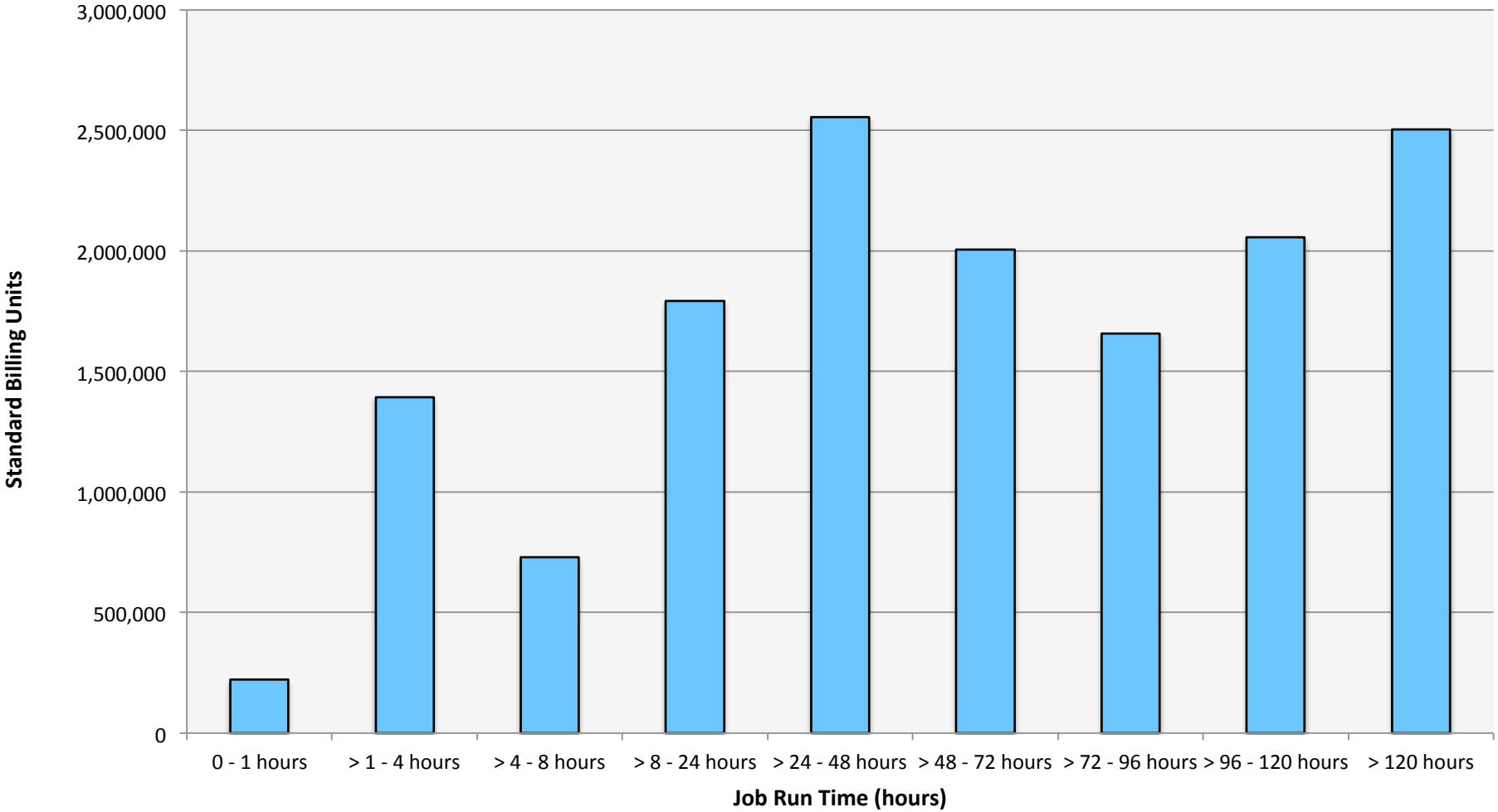
Pleiades:
SBUs Reported, Normalized to 30-Day Month



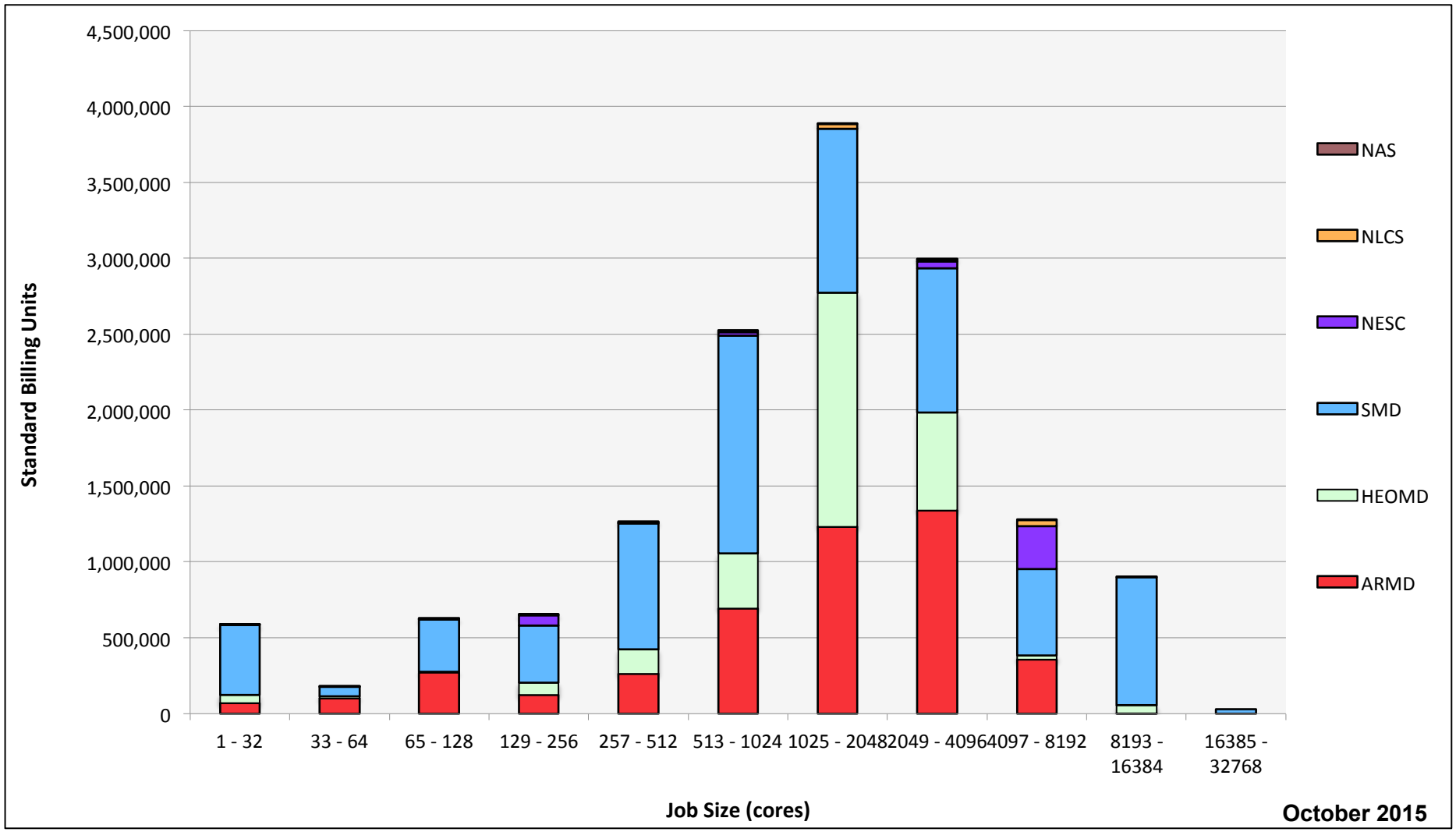
Pleiades:
Devel Queue Utilization



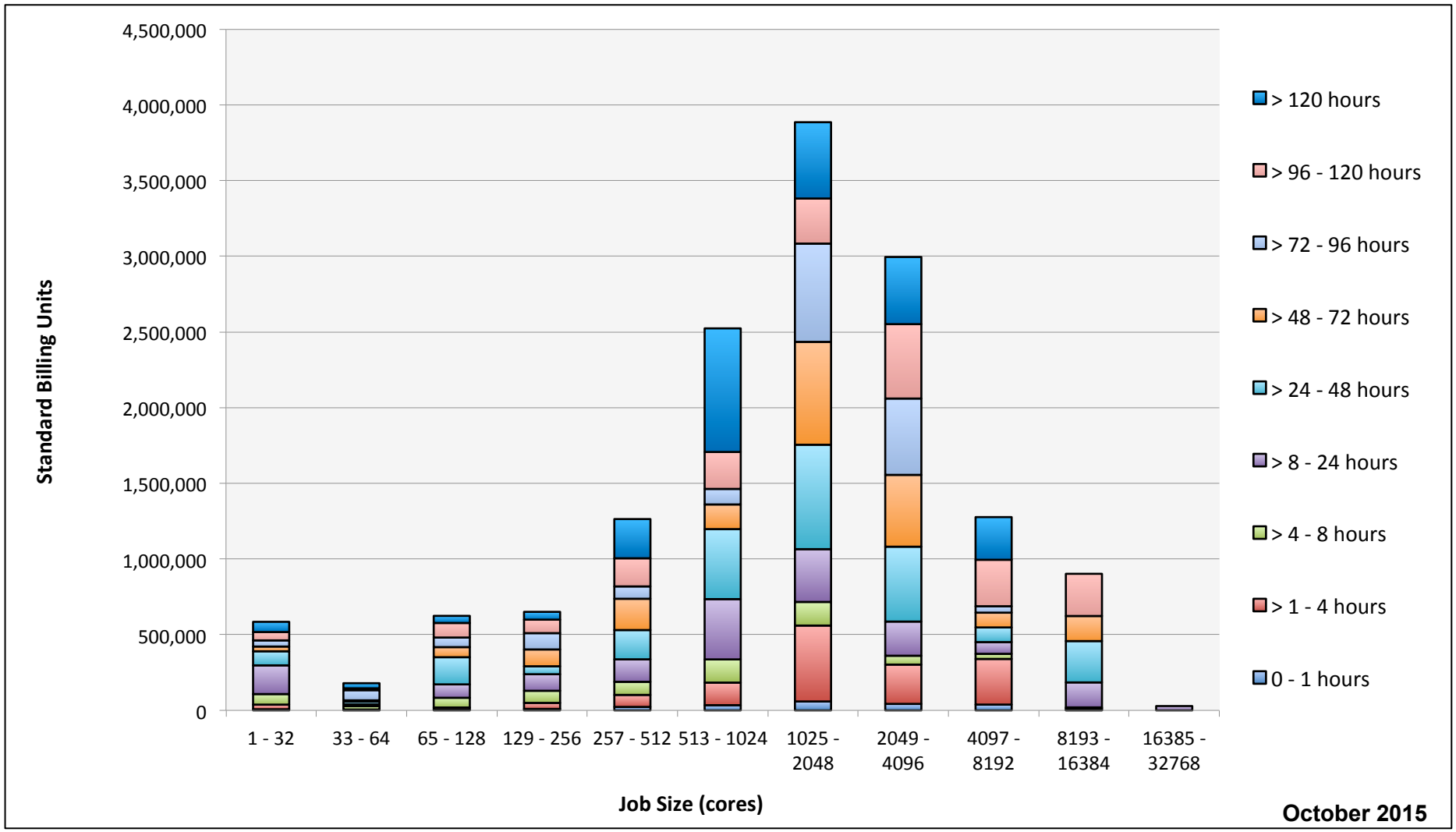
Pleiades:
Monthly Utilization by Job Length



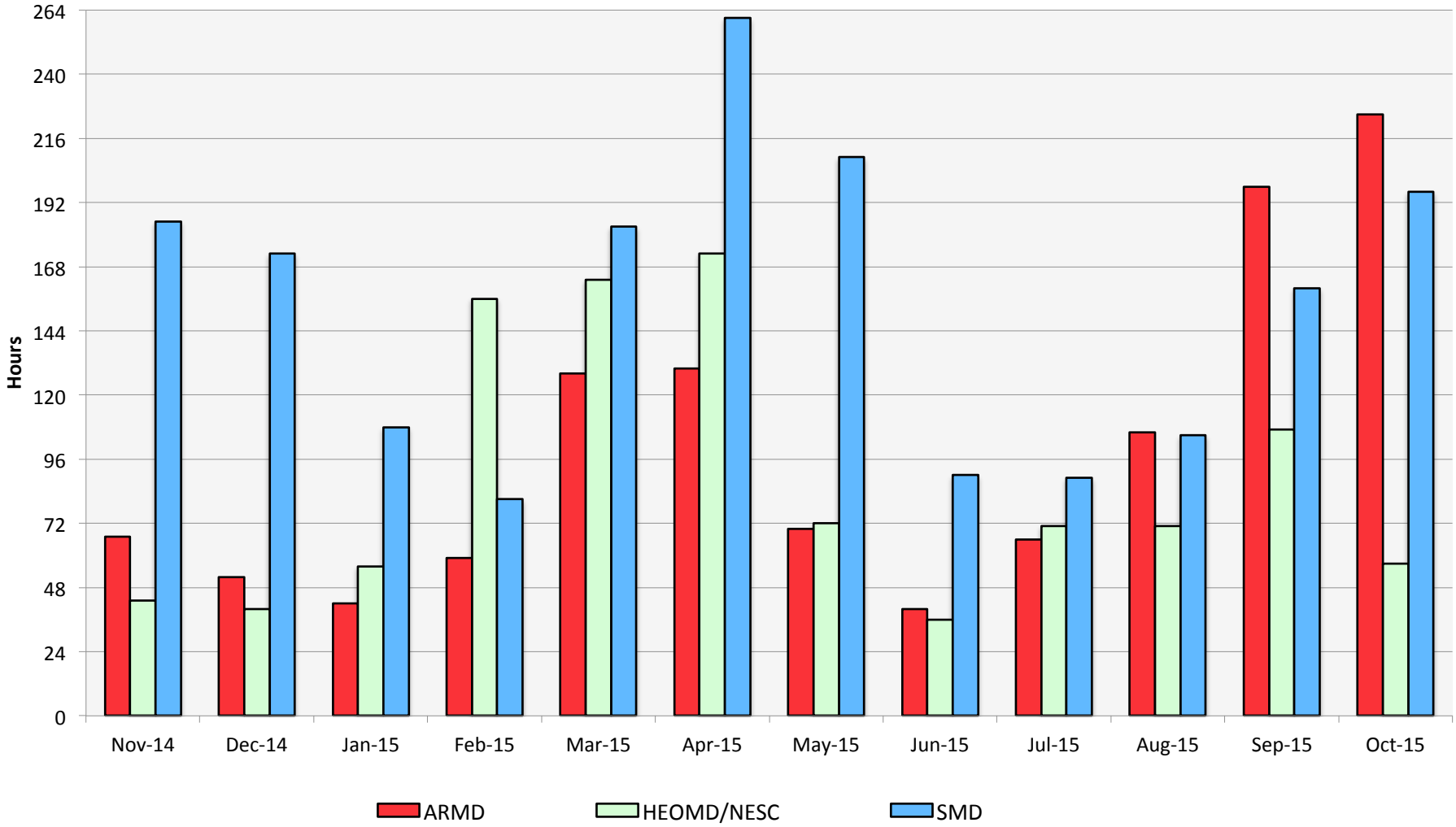
Pleiades:
Monthly Utilization by Size and Mission



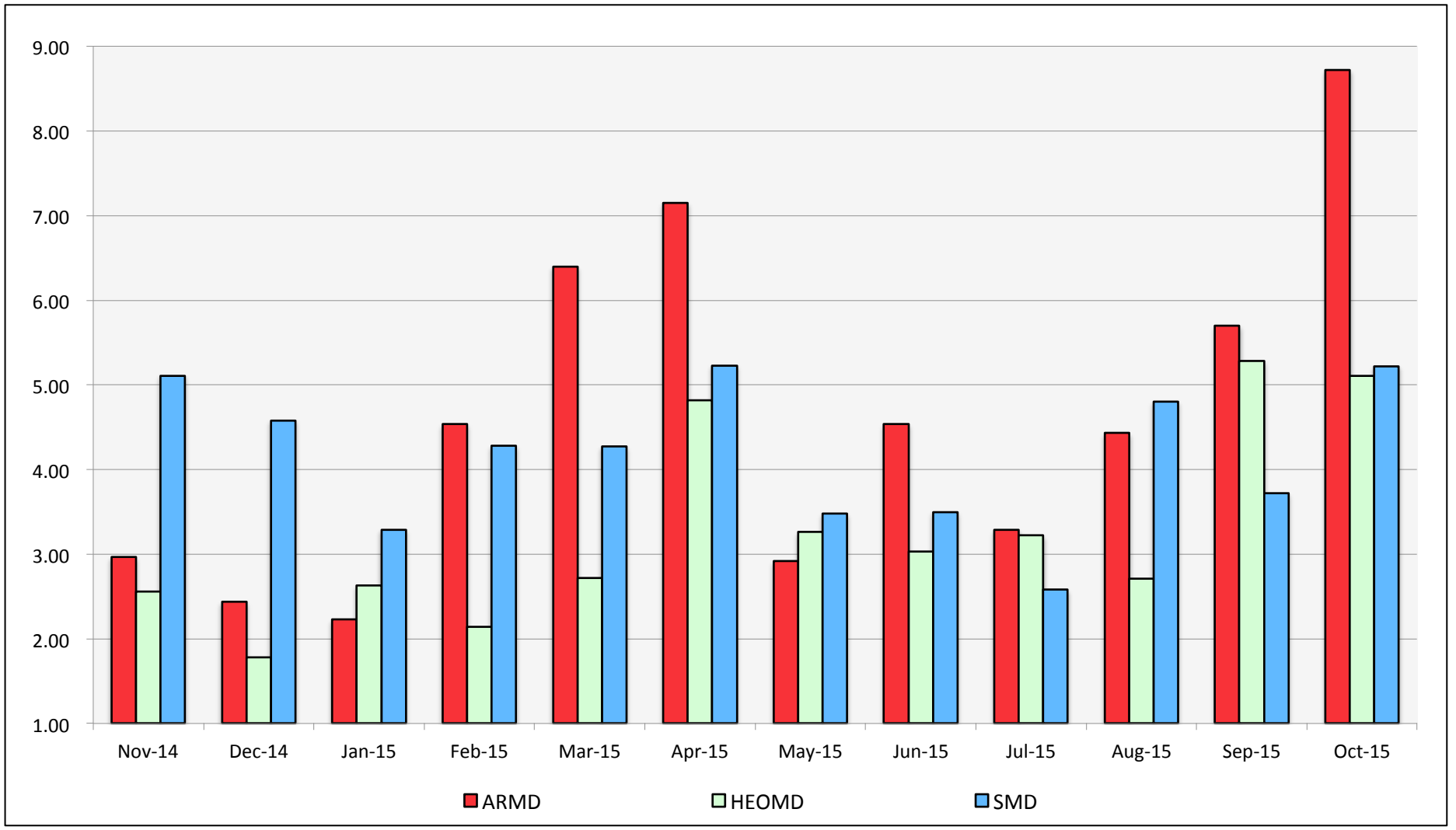
Pleiades:
Monthly Utilization by Size and Length



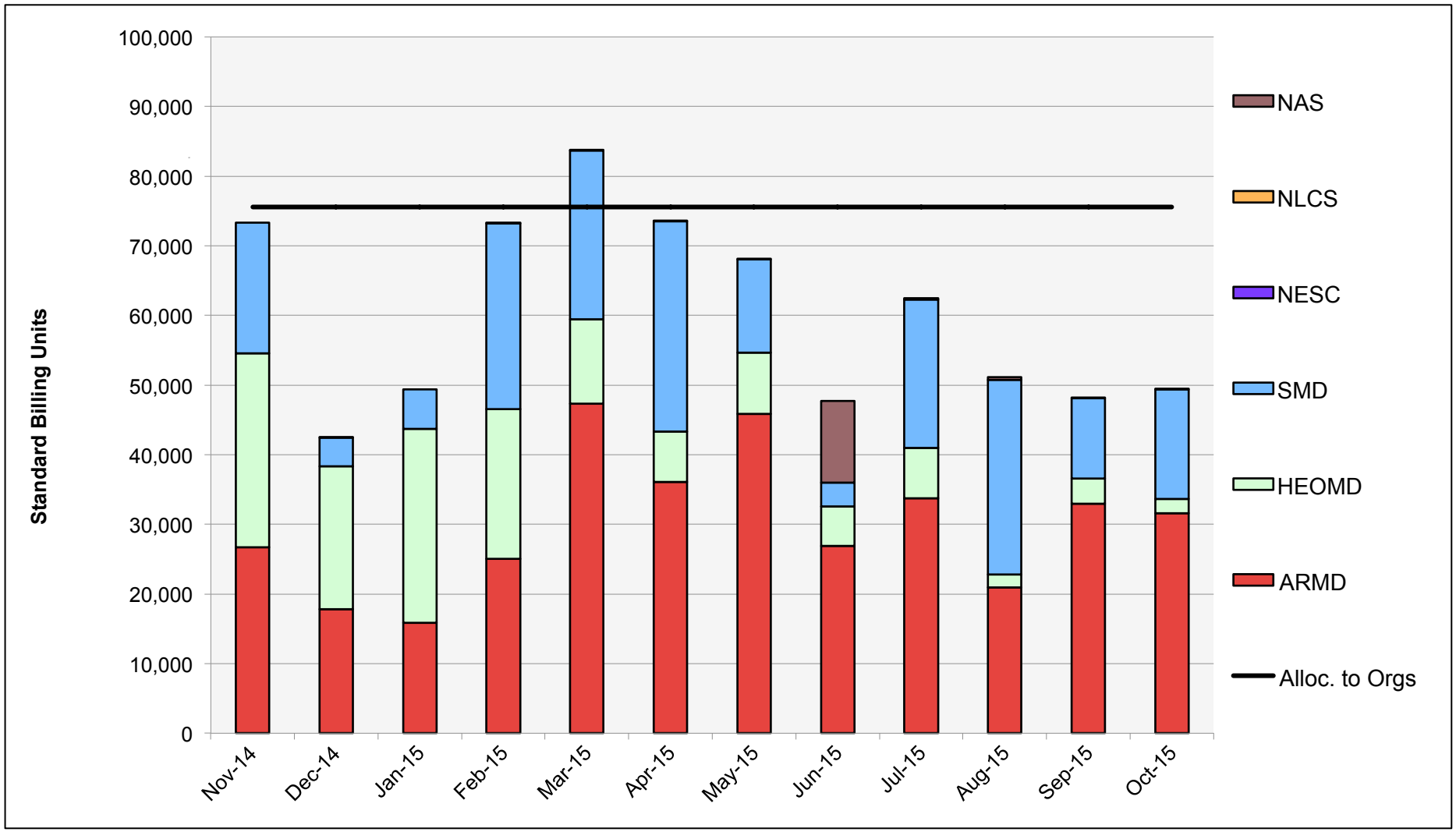
Pleiades:
Average Time to Clear All Jobs



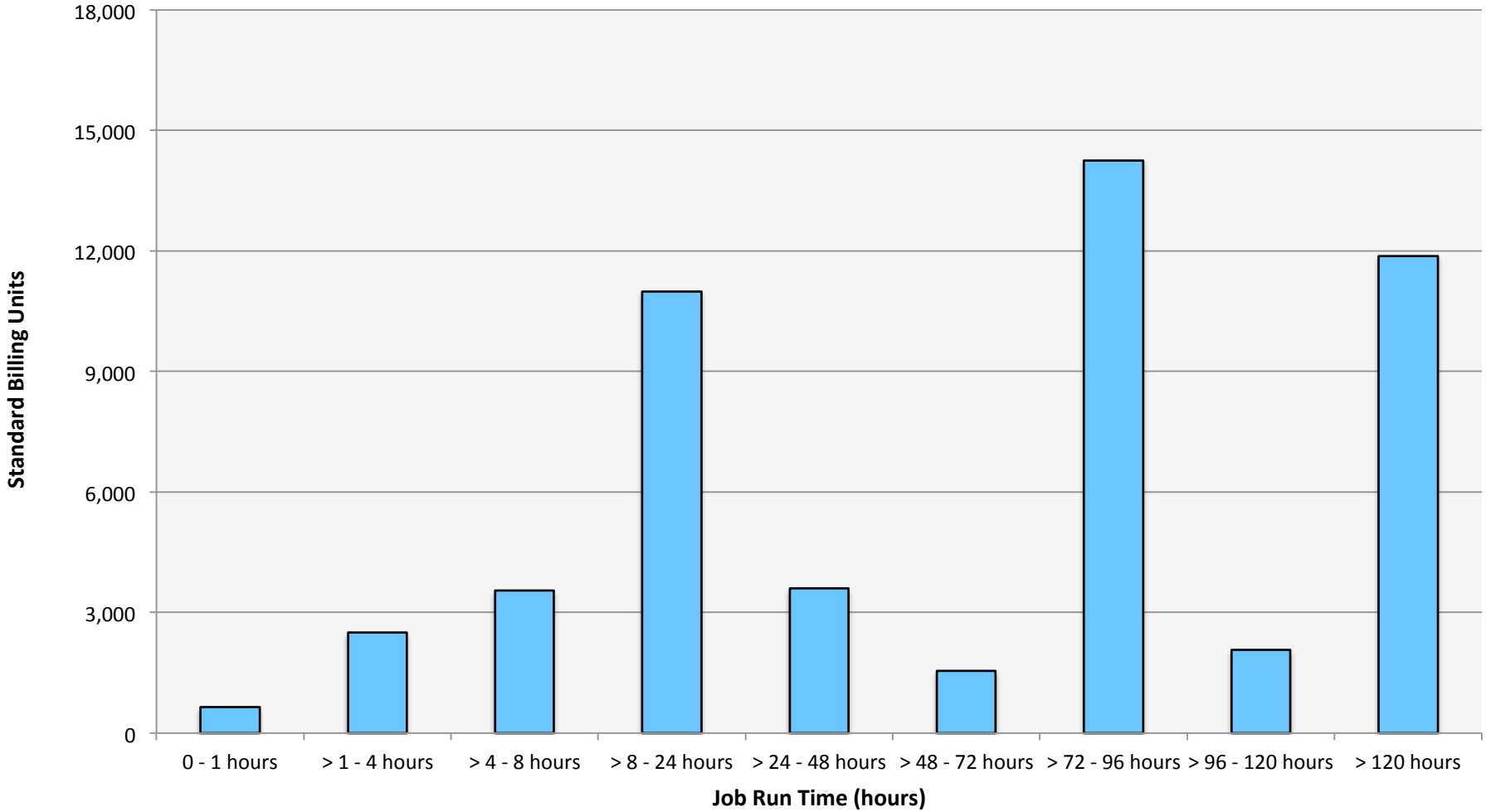
Pleiades:
Average Expansion Factor



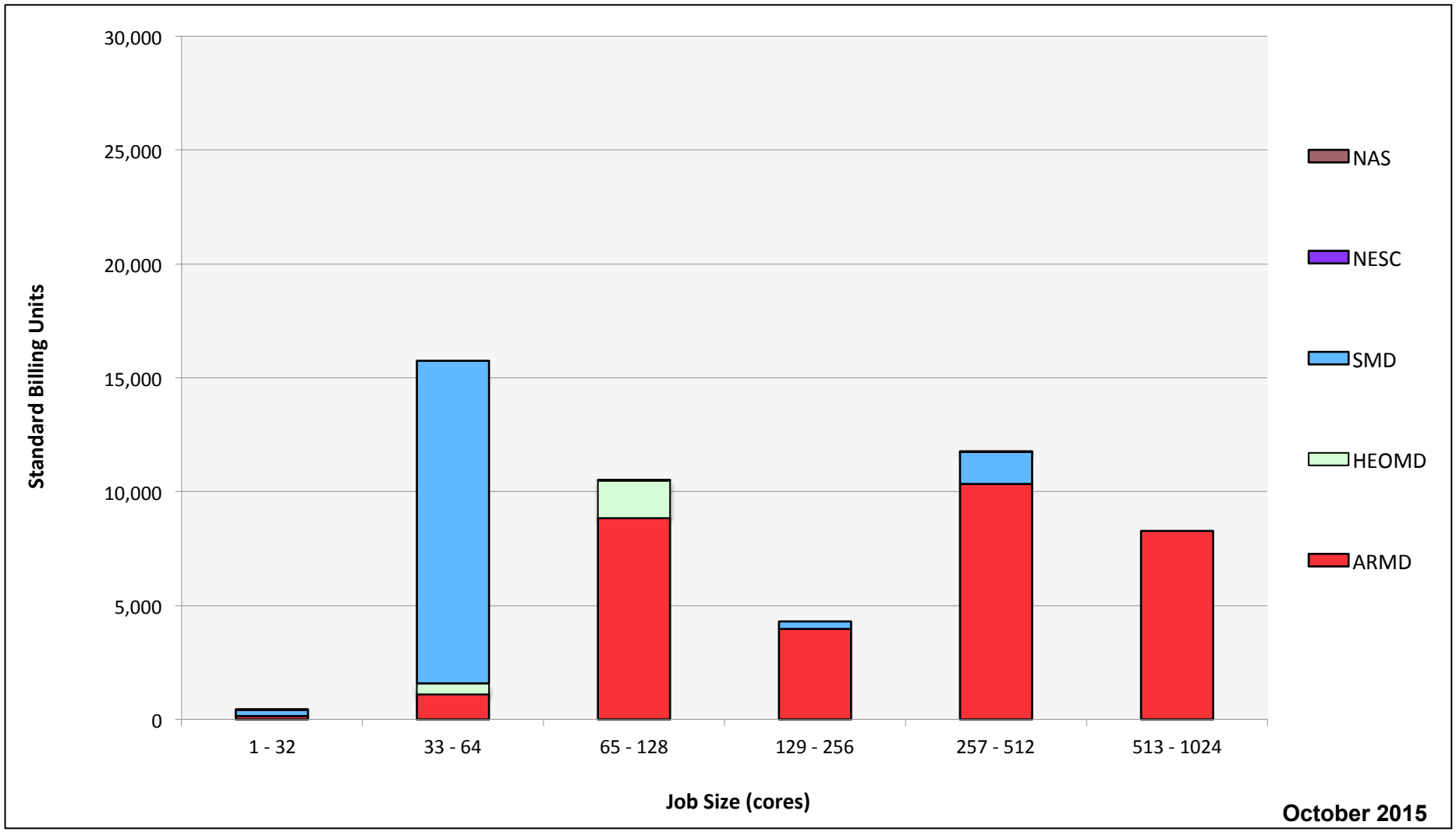
Endeavour:
SBUs Reported, Normalized to 30-Day Month



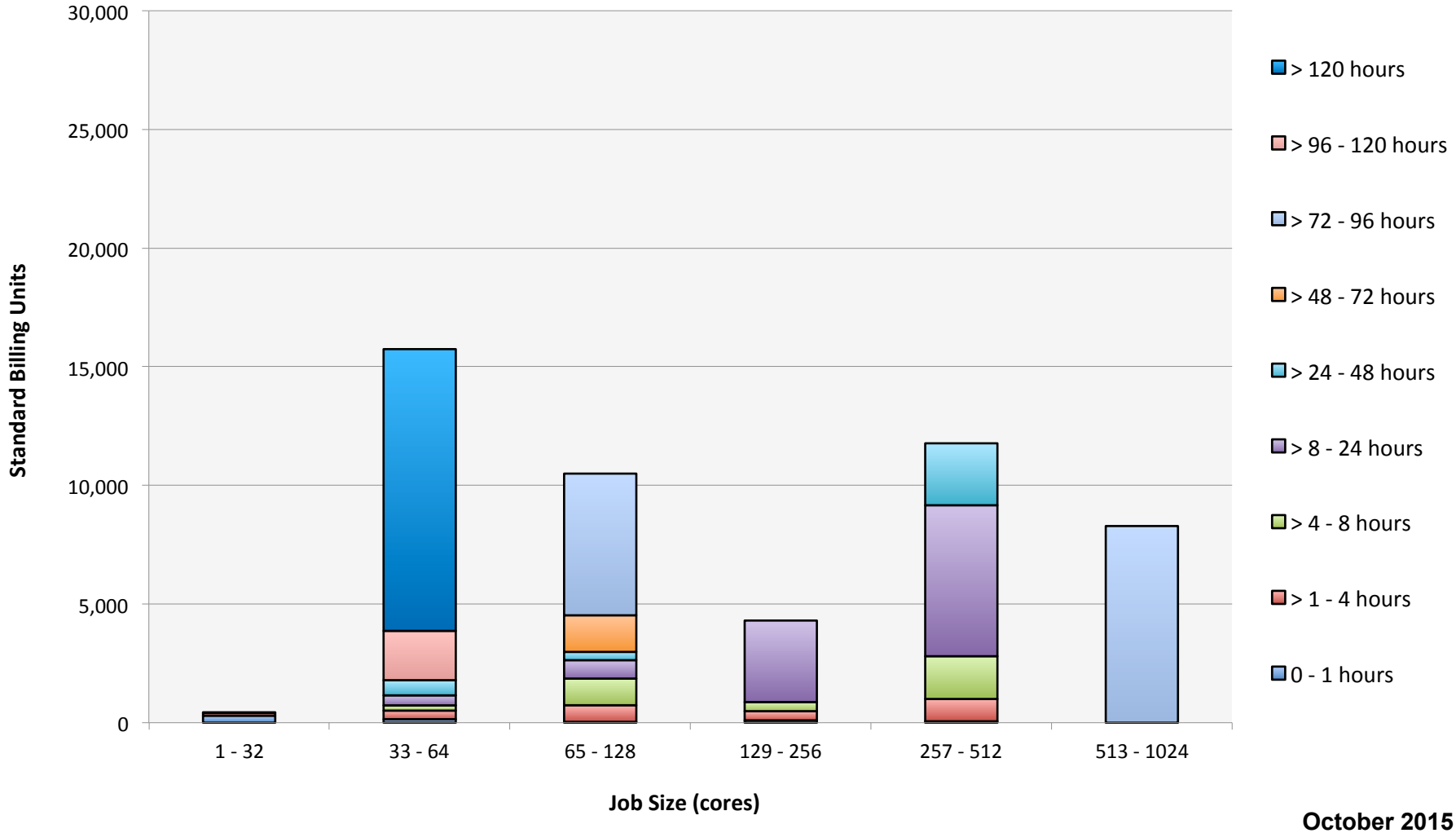
Endeavour:
Monthly Utilization by Job Length



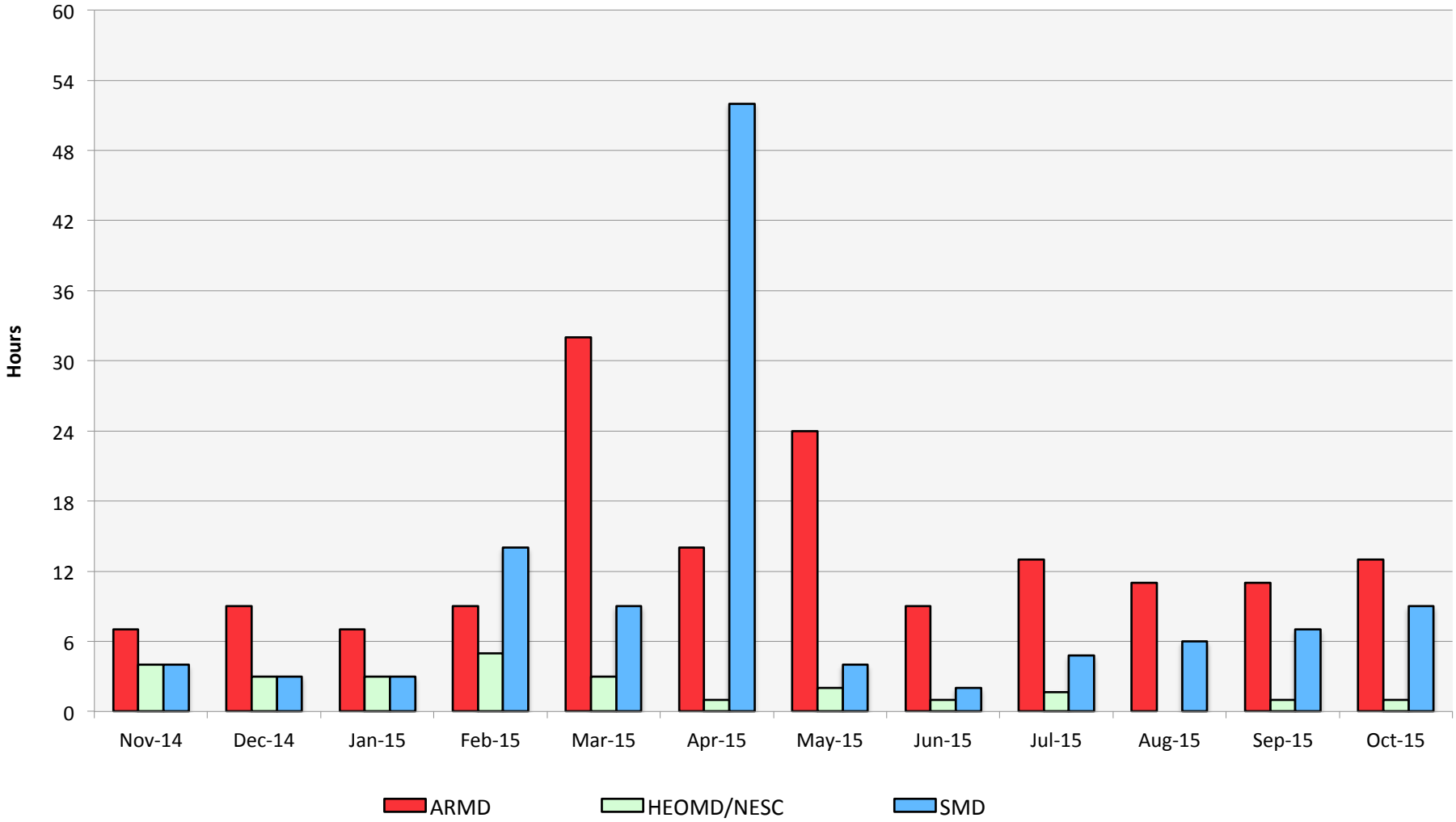
Endeavour:
Monthly Utilization by Size and Mission



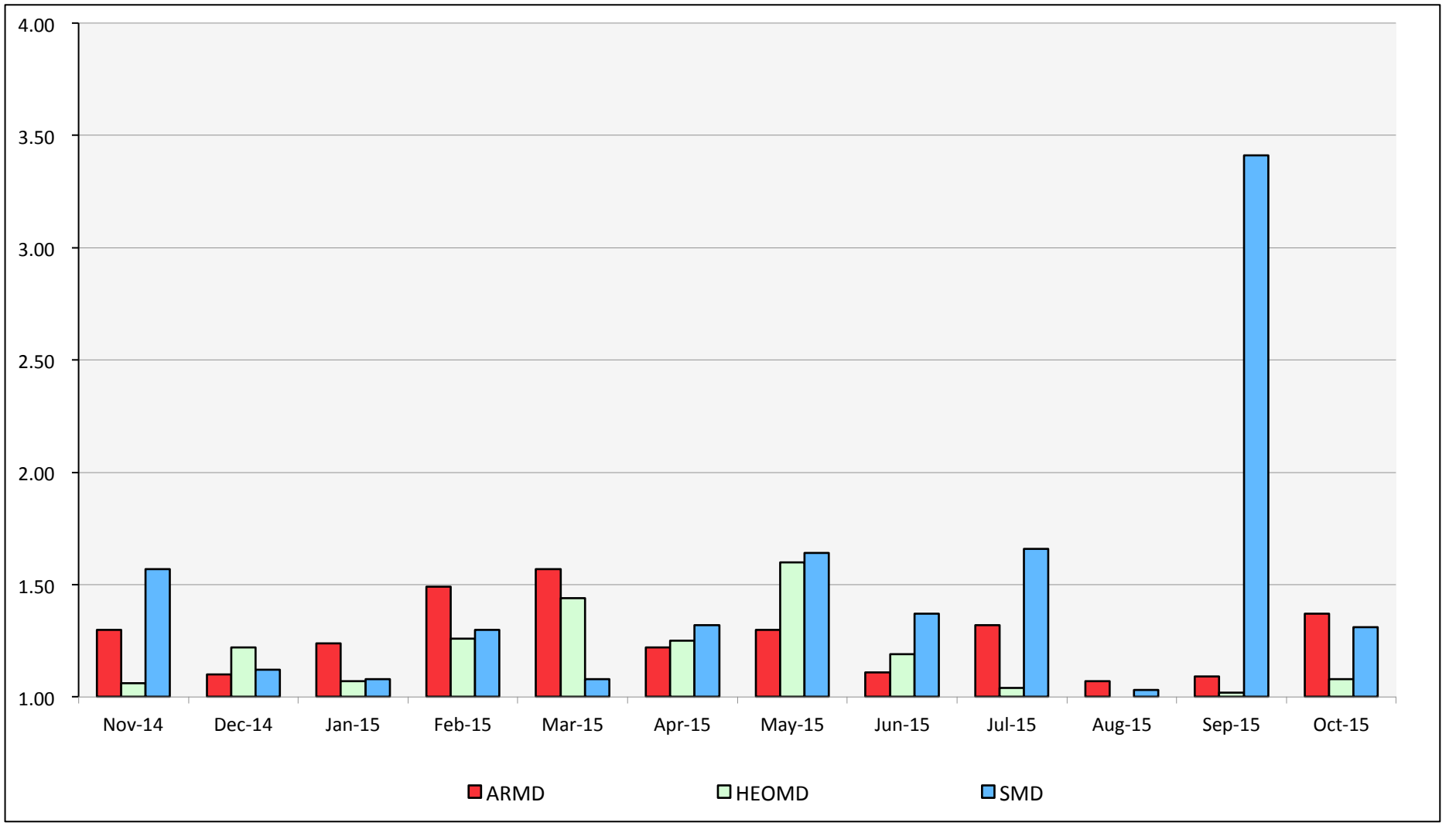
Endeavour:
Monthly Utilization by Size and Length



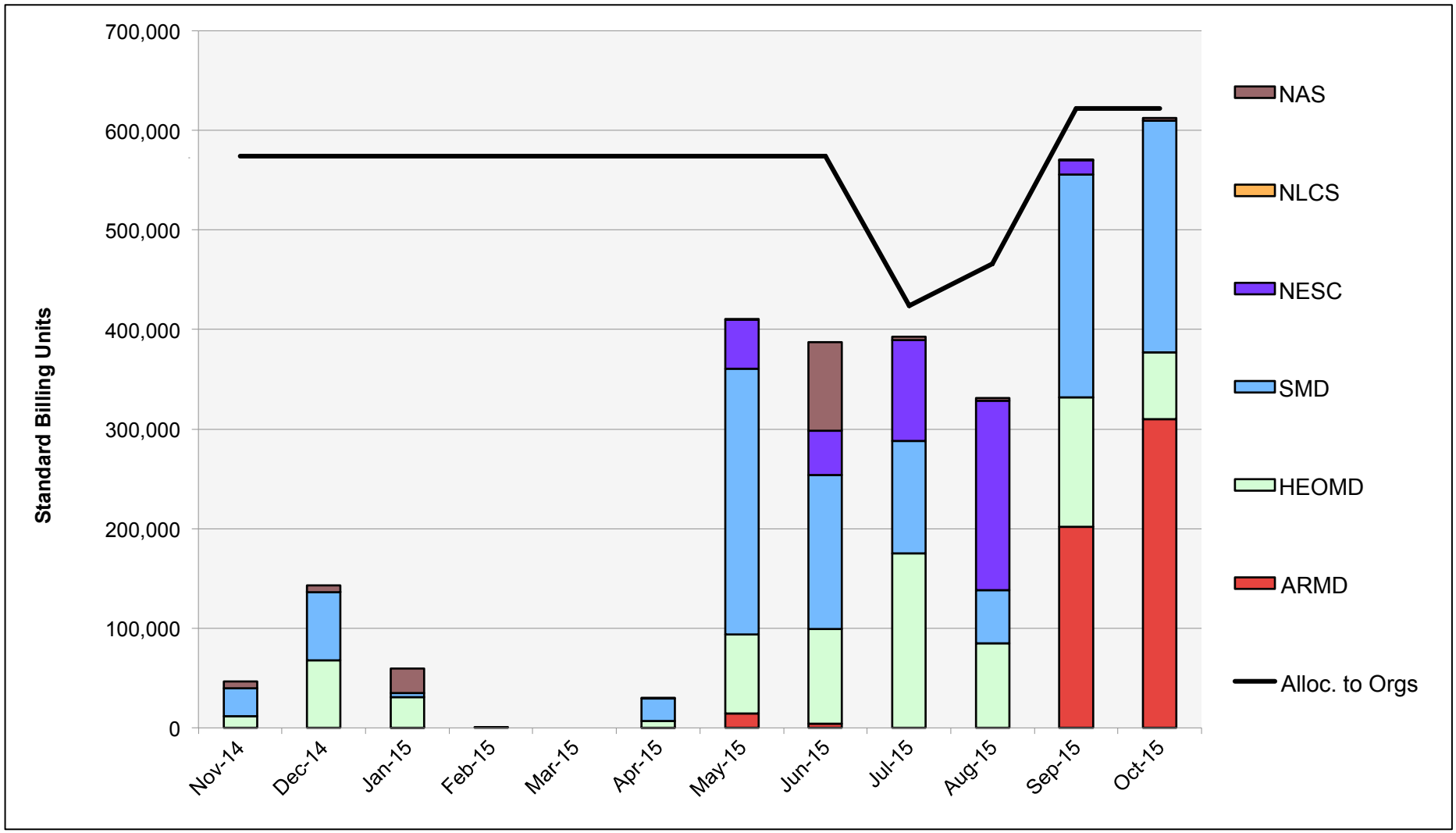
Endeavour:
Average Time to Clear All Jobs



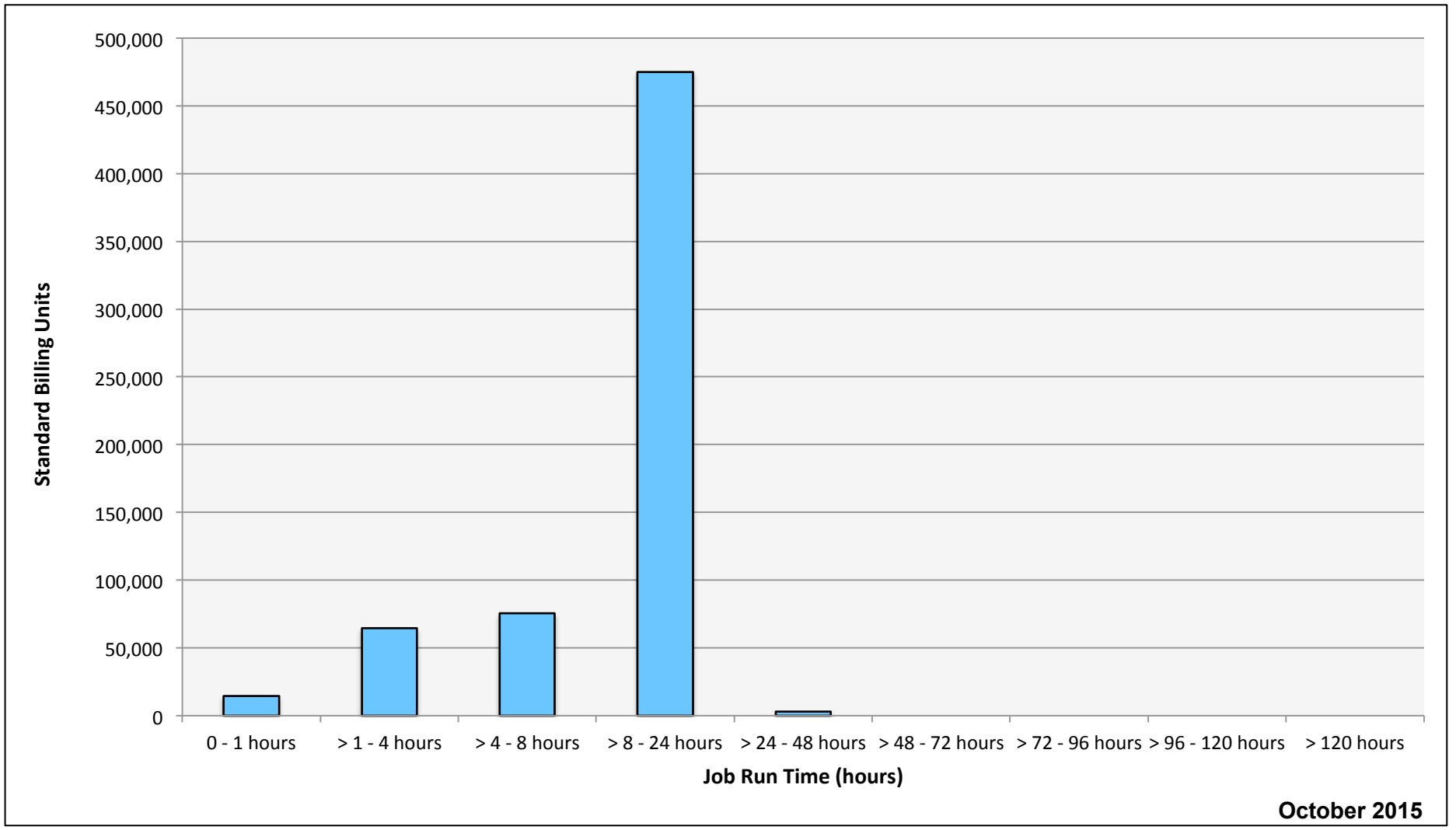
Endeavour:
Average Expansion Factor



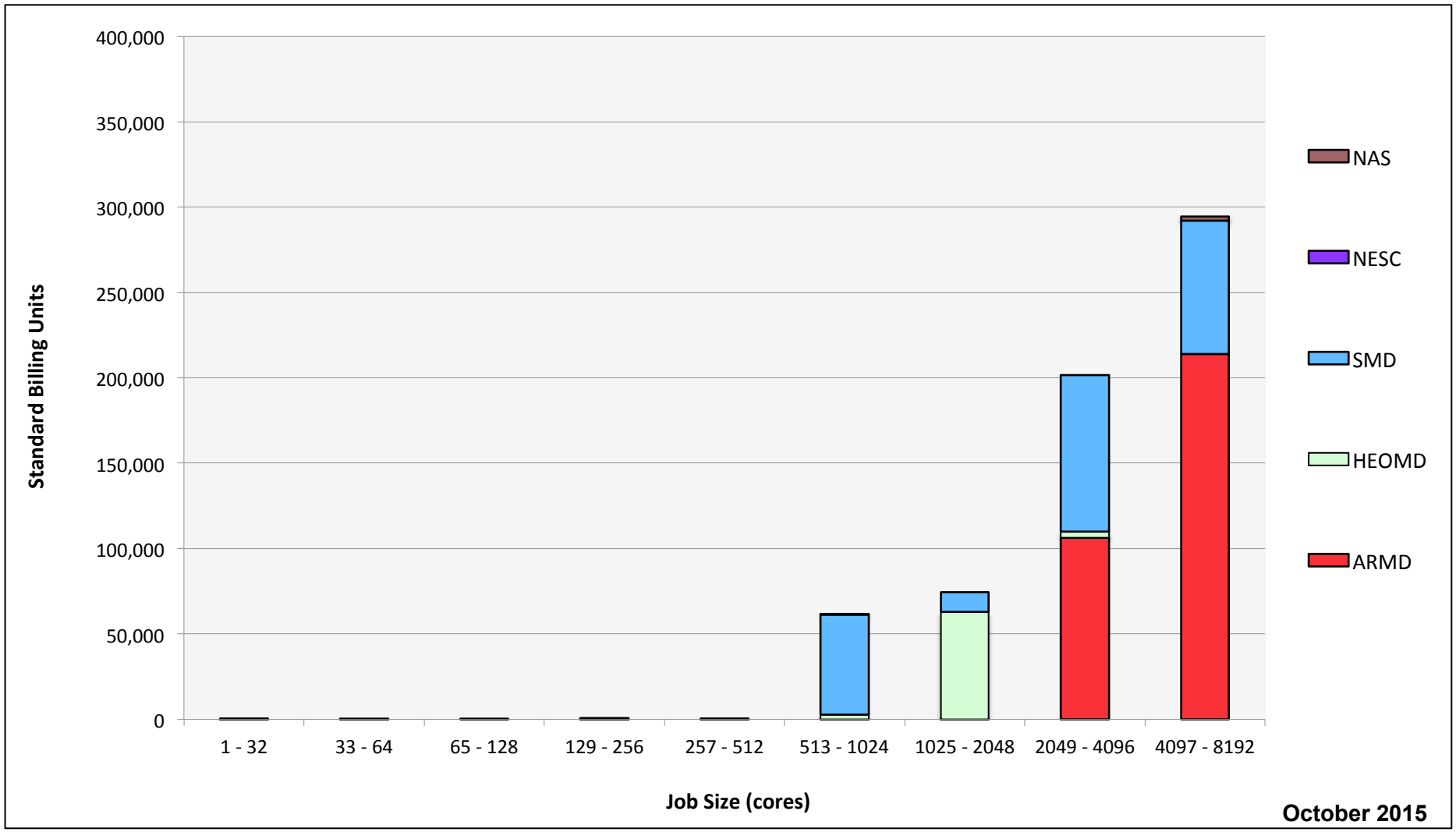
Merope:
SBUs Reported, Normalized to 30-Day Month



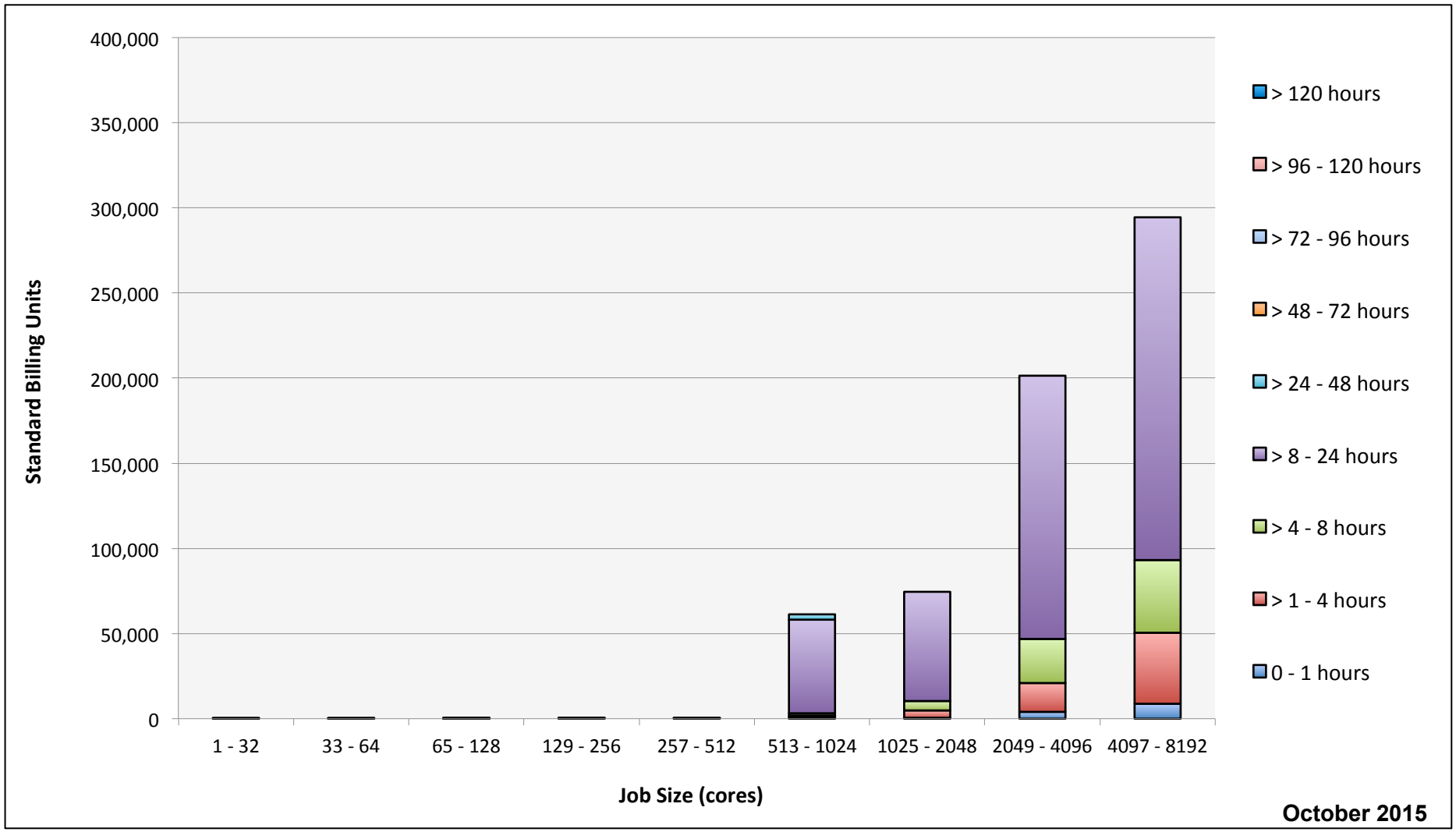
Merope:
Monthly Utilization by Job Length



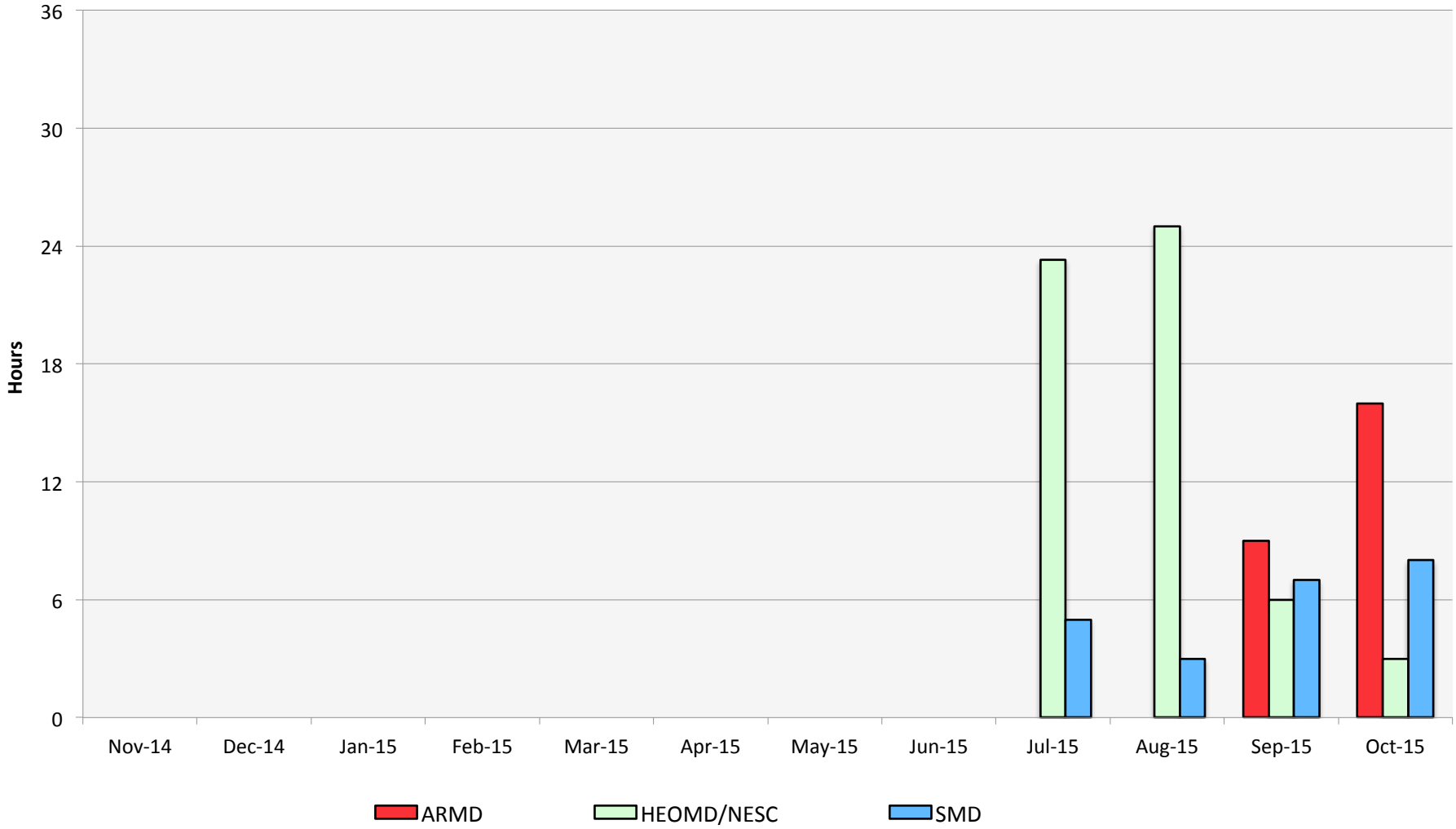
Merope:
Monthly Utilization by Size and Mission



Merope:
Monthly Utilization by Size and Length



Merope:
Average Time to Clear All Jobs



Merope:
Average Expansion Factor