Project Status Report

High End Computing Capability
Strategic Capabilities Assets Program

October 10, 2015

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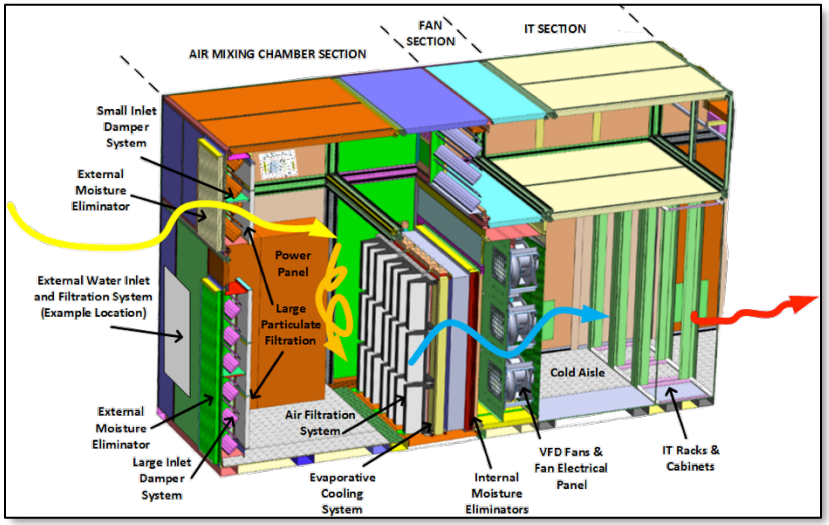
SGI Selected to Provide Prototype Modular High-Performance Computer Facility

- We received five proposals and selected SGI to provide a modular data center and initial Haswell-based compute nodes to study the effectiveness of a modular approach to HPC.
- The initial system, a Data Center on Demand (DCoD)-20 manufactured by CommScope, will be delivered by SGI with 288 Haswell nodes in 4 racks. The modular container can be expanded to 1,152 nodes in 16 racks.
- Utilizing adiabatic cooling technology, the container will take advantage of the temperate climate in the San Francisco Bay Area.
  - We estimate that, for the majority of the year, cooling will be provided with (filtered) outside air with no additional cooling required.
  - On the days when additional cooling *is* required, it will be done by passing water over a membrane using evaporation to cool the air.
  - This will result in a 99% reduction in water use and a 13% reduction in electric energy consumption compared to our current facility.
- After installation, we will conduct extensive tests to compare the water and electrical usage of this technology against the existing computer facility.

Mission Impact: A significant component of the cost to operate a computer center is the cost to cool it. By looking at alternatives to traditional computer floors, HECC can significantly reduce the impact to the environment while saving money for NASA.



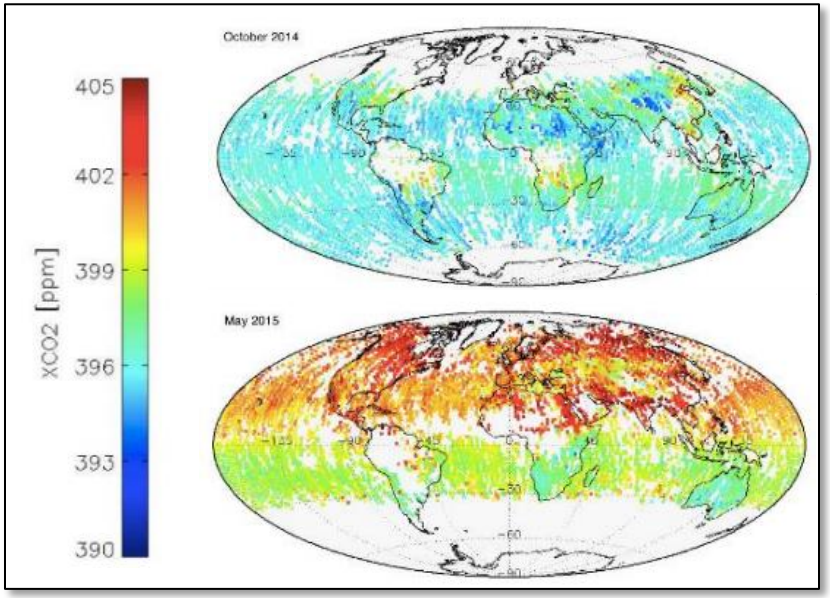
The Data Center on Demand (DCoD)-20 takes advantage of the mild climate in the San Francisco Bay Area. The air is brought in through filters on the exterior of the container and introduced into a mixing chamber. If required, water is run through the evaporative cooling media to drop the temperature of the air before it is used to cool the IT equipment. The hot air is then released back outside.

POC: William Thigpen, william.w.thigpen@nasa.gov, (650) 604-1061, NASA Advanced Supercomputing Division

Pleiades Enables OCO-2 Reprocessing for a Consistent Ten-Month Data Record

- Enabled by the extensive use of Pleiades, the Orbiting Carbon Observatory (OCO-2) team at JPL recently completed a major data reprocessing campaign covering ten months of the mission.
- About 60% of the campaign was pushed through Pleiades, including 18.6 million instrument soundings.
- Because the full physics retrieval process operates on the soundings independently to extract XCO_2, it is well suited to the Pleiades architecture. The JPL team utilized HECC's highly reliable transfer tools, up to 500 Pleiades' Haswell nodes, and 1.4 million processor-hours.
- The added computing resources allowed the team to complete the campaign about 3 months sooner than initially planned; and get a consistent, well-calibrated, and comprehensive dataset out to the public quickly.
- Science team members and the larger community are now mining the data record at both global (see maps at right) and regional scales.

Mission Impact: Using the Pleiades supercomputer, scientists completed data reprocessing for the OCO-2 mission three months ahead of schedule. The improved dataset will help the science community understand how human-produced greenhouse gas drives changes in Earth's climate.



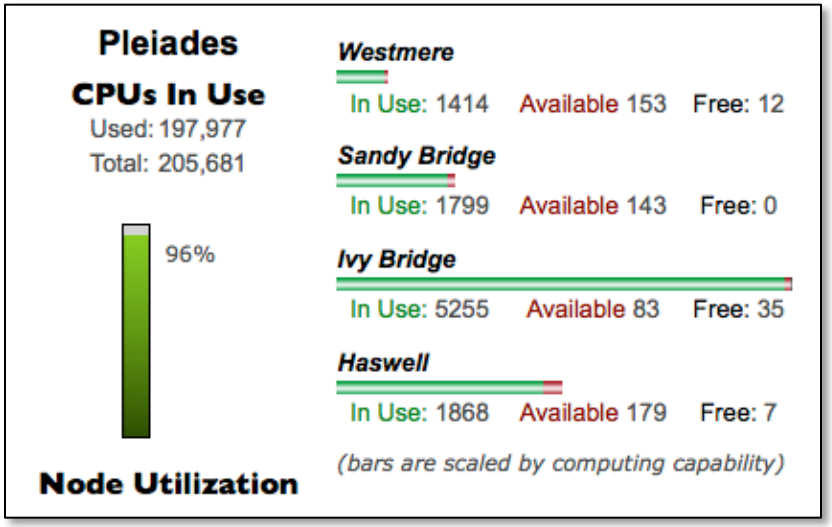
Global XCO_2 maps for October 2014 and May 2015.

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

PBSPro Configuration Changes Improve Scheduling Performance

- HECC Supercomputing Systems staff, in collaboration with vendor Altair, achieved a 5 times improvement in PBSPro job scheduling performance for Pleiades.
- Based on information shared between HECC and Altair, and analysis conducted by Altair on scheduler performance bottlenecks, our Systems staff made configuration changes to job scheduling on Pleiades.
  - We had previously selected a feature in the scheduler that looked at the node type to reduce the scheduling load. Altair had separately sped up the scheduler when this feature wasn't used. By no longer selecting the feature we saw significant improvement overall.
  - The second improvement involved the order of code execution. By changing the order we significantly reduced the number of operations executed.
- We expect further significant improvement in job scheduling performance from upcoming work related to scheduling algorithm design (see slide 6).

Mission Impact: Improvements in job scheduling performance assist system engineers in keeping the HECC computational capability as fully utilized as possible.



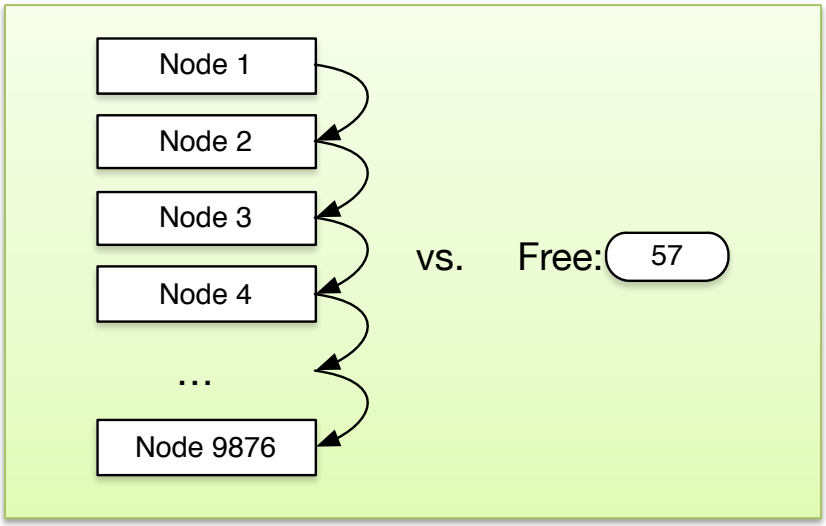
HECC staff maintain Pleiades supercomputer utilization at 90-plus percent, with the help of a well-performing scheduler. Job requests are matched with free nodes according to a scheduling policy that ensures fairness for missions, groups, and users.

POCs: Greg Matthews, gregory.a.matthews@nasa.gov (650) 604-1321, and Dale Talcott, dale.r.talcott@nasa.gov, (650) 604-0555, NASA Advanced Supercomputing Division, Computer Sciences Corp.

Systems Experts Design New Pleiades Job Scheduling Algorithm

- In addition to PBSPro configuration changes (see slide 5), HECC Supercomputing Systems staff designed a new algorithm that should significantly speed up job scheduling for Pleiades.
- The current job scheduling algorithm involves many searches of long lists of nodes. This technique can perform well for moderate-sized clusters, but superclusters like Pleiades require a different approach.
- The new algorithm spends a little additional time up front categorizing nodes into "buckets" of similar nodes. This streamlines the remaining steps in the algorithm, improving performance and enabling the use of additional scheduling features.
- The PBSPro vendor, Altair, was tasked with generating a prototype matching the design to allow us to evaluate the effectiveness of the algorithm.

Mission Impact: A new algorithm for scheduling the work done on the Pleiades supercomputer better tailors the scheduler to the system's characteristics, improving utilization of the HECC computational capability.



Searching a list of nodes to find information while scheduling jobs—compared with aggregating information in advance—is computationally much more expensive on a large system like Pleiades.

POCs: Dale Talcott, dale.r.talcott@nasa.gov, (650) 604-0555, and Greg Matthews, gregory.a.matthews@nasa.gov (650) 604-1321, NASA Advanced Supercomputing Division, Computer Sciences Corp.

Video Enhancement Enables Analysis of ISS Experiment Videos

- HECC Visualization experts enhanced videos of a fruit fly experiment recorded onboard the International Space Station (ISS) to allow scientific analysis.
- Visualization staff produced the enhancement to simplify the background enabling the science team to use an open-source tool, CTRAX, to track the fruit flies.
- The enhancement included:
  - Determining the background by looking at the entire video and finding—for each pixel—the color that occurs most often.
  - Subtracting the background from each video frame, and then increasing the contrast of the frames.
- The same enhancement approach will be used with a ground control experiment to be done at the end of CY2015.
- "The video enhancement work … has been instrumental in allowing us to analyze our spaceflight videos" – Sharmila Bhattacharya, principal investigator.

Mission Impact: HECC's scientific visualization capability enabled better data analysis of an experiment taking place on the International Space Station.

Left: Excerpt from an original fruit fly video recorded onboard the ISS.
Right: Processed video with the background subtracted and with the contrast enhanced. The white objects are moving fruit flies. The videos are shown 5x normal speed.

POC: David Ellsworth, david.ellsworth@nasa.gov, (650) 604-0721, NASA Advanced Supercomputing Division, Computer Sciences Corp.

Staff and Users Trained on OpenACC Approach to GPU Parallelization

- In early September, two dozen HECC staff members and scientists from ARC and LaRC attended a two-day training session on OpenACC provided by GPU vendor NVIDIA.
  - OpenACC is a programming standard for offloading programs from a host CPU to an attached accelerator device, such as a GPU.
  - Similar to the OpenMP application programming interface, OpenACC is directive based, which makes it easier for application developers to convert their existing CPU-centric codes for running on GPUs, compared to the language-based Compute Unified Device Architecture (CUDA) approach.
- In addition to a day of presentation, NVIDIA personnel provided one-on-one help for attendees on day two.
- The lab experience helped HECC scientists better identify candidate applications for running on the GPUs. One such example is the Launch Ascent and Vehicle Aerodynamics (LAVA) acoustic scattering code, which shows impressive speedup with OpenACC compared to a serial version. Other applications, such as the Chimera Grid Tools, will require more effort.

Mission Impact: Familiarity with OpenACC allows HECC staff to help user applications take advantage of existing GPU resources on Pleiades—a potentially huge productivity boost over conventional processors.

The Pleiades supercomputer includes 64 nodes with Intel Sandy Bridge processors and NVIDIA K40 graphics processing units (GPUs), and 64 nodes with Intel Westmere CPUs and NVIDIA M2090 GPUs.

POCs: Robert Hood, robert.hood@nasa.gov, (650) 604-0740, NASA Advanced Supercomputing (NAS) Division, Computer Sciences Corp.; Cetin Kiris, cetin.c.kiris@nasa.gov, (650) 604-4485, NAS Division

HECC Successfully Completes Annual Inventory for 2015

- The HECC Property group successfully completed the 2015 annual equipment inventory of 1,284 pieces of equipment, with a 99.5% scan rate.
- Six items were not located. To close out these items, Property Survey Reports (Form NF598) were completed to identify the assets as missing equipment and remove them from the NASA property database.
- The Property staff's active tracking and updating of the HECC/NAS data helped ensure a successful inventory. Ongoing tracking and management of equipment during FY15 included:
  - Tagging 142 new pieces of equipment.
  - Excessing 97 pieces of equipment.
  - Responding to 850 Remedy tickets, most of which were requests for updates to equipment location and ownership.

Mission Impact: Accurate tracking of assets through their life cycle, and removal of NASA data prior to system disposal, ensures control of government equipment and prevents loss of NASA data.

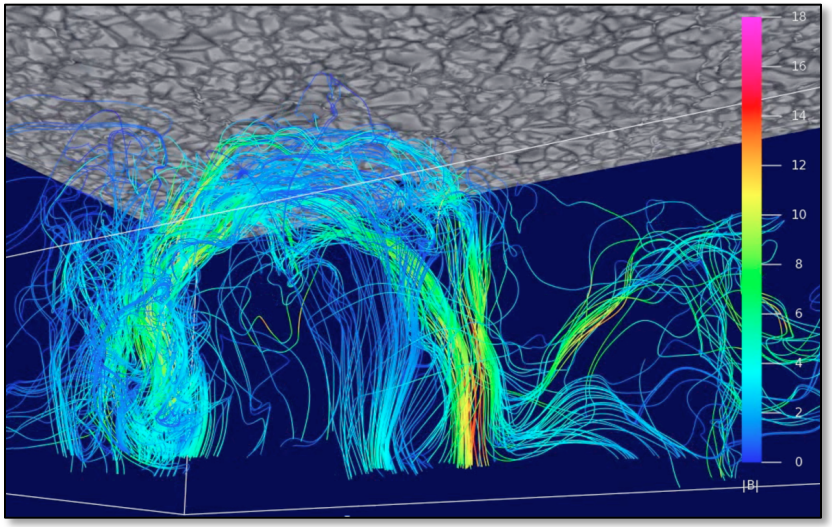
During the annual equipment inventory, HECC property custodians account for all equipment associated with the NASA Advanced Supercomputing (NAS) facility, including all components of the Pleiades supercomputer.

POC: Cathy Parks, cathy.b.parks@nasa.gov, (650) 604-4314, NASA Advanced Supercomputing Division, Computer Sciences Corp.

Magnetohydrodynamic Simulations to Understand the Sun's Weather

- Researchers in the Physics and Astronomy Department at Michigan State University (MSU) are using Pleiades to model solar-magneto convection, supporting NASA's goal to understand how the Sun's weather interacts with Earth and the solar system.
- The MSU magnetohydrodynamic simulations reveal:
  - Convective motions transport heat and act as a dynamo, strengthening the magnetic field by stretching and twisting it.
  - As the magnetic field approaches the solar surface, violent convective motions keep the large-scale structure intact while simultaneously shredding the field into thin filaments.
  - As a result of these motions, active-region magnetic fields emerge with mixed polarities, which then counterstream to collect into opposite-polarity pores and sunspots.
- Using Pleiades allows the researchers to include the interactions of disparate spatial and temporal scales of motion. In this case, spatial scales ranged from solar supergranules (48,000 kilometers) to sub-granules (24 km).
- HECC visualization services are also essential to understanding these complex phenomena.

Mission Impact: Models of solar-magneto convection improve diagnostics that will help achieve NASA's goal of predicting the emergence of magnetic fields before they become visible at the solar surface.



Visualization of magnetic field lines at the point where a large loop (25 megameters wide) approaches the Sun's surface. Convection has kept the overall loop structure coherent while shredding it into thin filamentary fields. Colors show field strength from low (blue) to high (magenta). *Patrick Moran, NASA/Ames*

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

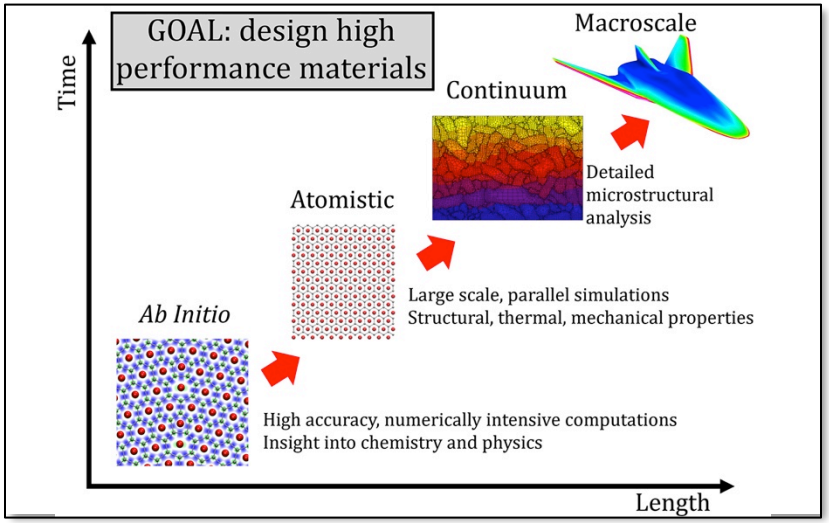
POC: Robert Stein, stein@msu.edu, (517) 884-5613, Michigan State University

Modeling Materials: Design for Planetary Entry, Electric Aircraft, and Beyond *

- Researchers at NASA Ames are performing multiscale modeling on Pleiades to aid development of new materials used in vehicle construction and to provide insight into existing ones.
- Multiscale modeling connects computational methods ranging from the atomic level to the macroscale. The output of one level is passed on as input to the next level, creating a powerful predictive model.
- The first level is quantum mechanical, probing a material's chemistry. At the next level, interatomic potentials, thermal and mechanical properties are determined. The final level, continuum modeling, inputs the atomic data and produces micro- and macroscale properties.
- Materials modeled include:
  - Ultra-high-temperature ceramics for hypersonic aircraft.
  - Ablative composites for planetary entry heat shields.
  - Advanced electrolytes for ultra-high-energy capacity batteries to be used in electric aircraft.
  - Shape-memory alloys for high-efficiency aircraft.
- Quantum mechanical and atomistic calculations are computationally intensive; modeling requires large cells, dense calculation meshes, and very long run times on Pleiades.

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

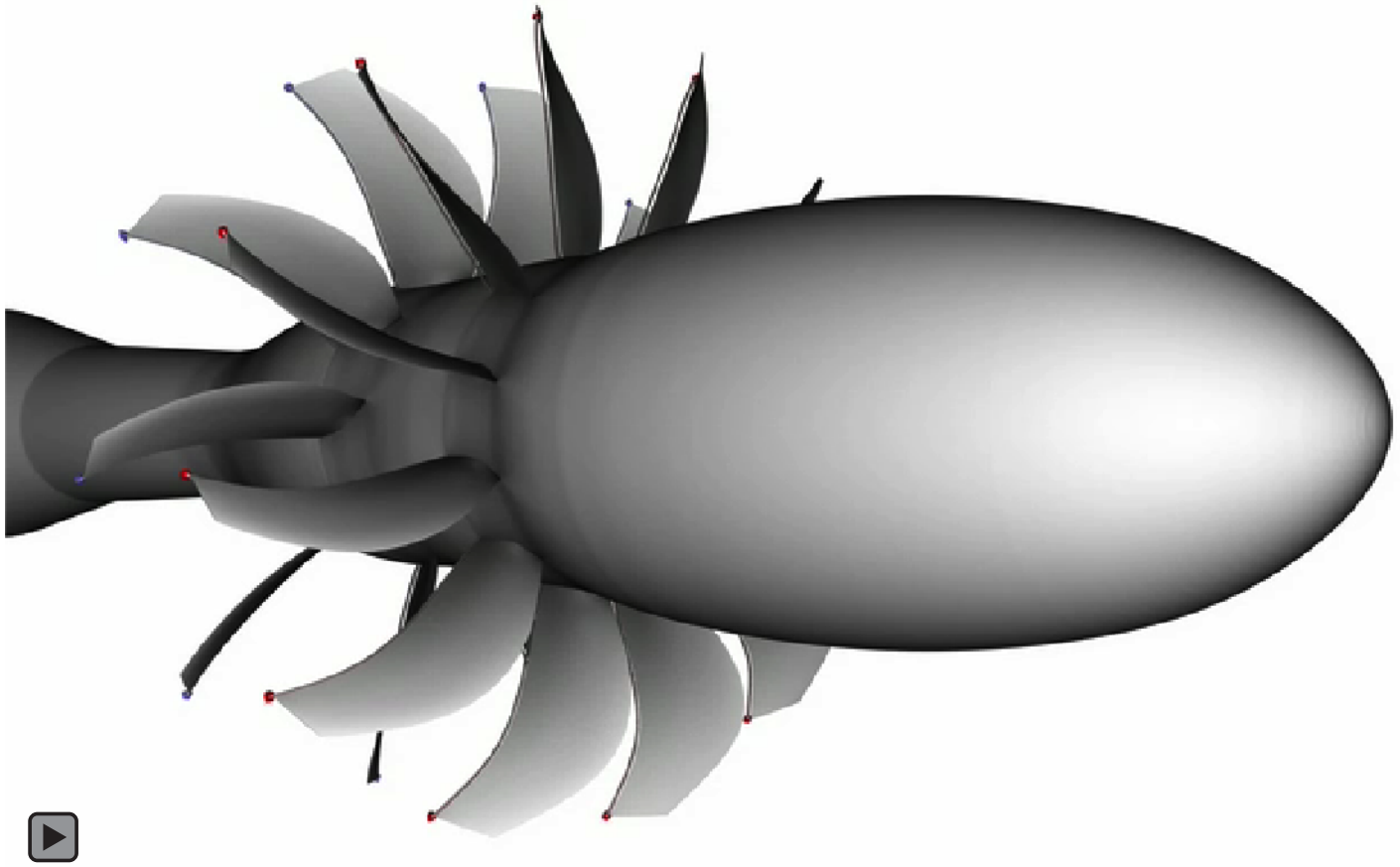
Mission Impact: Multiscale modeling helps NASA researchers develop the advanced, high-performance materials needed to design and build next-generation aircraft and space vehicles for the agency's projects and missions.



Multiscale modeling breaks down the elements of material design factors to their relevant time and length scales. As shown in the chart, the output of one level is passed on to the next level, creating a powerful predictive model.

POC: John Lawson, john.w.lawson@nasa.gov, (650) 604-6189, NASA Ames Research Center

Passive Particle Visualization of the Open Rotor Configuration Using LAVA



Passive particle visualization of contra-rotating, open-rotor simulation using the LAVA Cartesian higher-order accurate computational fluid dynamics (CFD) solver. Red particles are seeded on upstream blades, blue on aft blades. Solid colors are seeded on the tips, with faded colors on the blade trailing edges. ***POCs**: Michael Barad, michael.f.barad@nasa.gov, (650) 604-0550 and Cetin Kiris, cetin.c.kiris@nasa.gov, (650) 604-44l85, NASA Advanced Supercomputing (NAS) Division; Visualization: Timothy Sandstrom, NAS Division, Computer Sciences Corp.*

HECC Facility Hosts Several Visitors and Tours in September 2015

- HECC hosted 13 tour groups in September; guests learned about the agency-wide missions being supported by HECC assets; some groups also viewed the D-Wave Two quantum computer system. Visitors this month included:
  - A senior-level group from the U.S. Army Tank Automotive Research, Development and Engineering Center (TARDEC), who were meeting with ARC management for possible collaborations.
  - Andy David, the Consul General of Israel to the Pacific North West, as part of an ARC tour.
  - Attendees of the agency-wide Astrophysics Program Manager Quarterly Review.
  - Anja Fourie, Scifest Africa Director, accompanied by NASA Deputy Chief Technologist Jim Adams.

Participants in NASA-wide Astrophysics Program Manager Quarterly Review were treated to an overview of the HECC project and tour of the NASA Advanced Supercomputing (NAS) facility from Bryan Biegel, deputy chief of the NAS Division.

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

Papers

- "**Influence of Measurement Uncertainties on Soluble Aerosol Iron Over the Oceans**," N. Meskhidze, M. Johnson, D. Hurley, K. Dawson, Biogeosciences Discussions, vol. 12, September 1, 2015. *
  http://www.biogeosciences-discuss.net/12/14377/2015/bgd-12-14377-2015.html
- "**The Competition Between Lorentz and Coriolis Forces in Planetary Dynamos**," K. Soderlund, A. Sheyko, E. King, J. Aurnou, Progress in Earth and Planetary Science (Springer), September 2, 2015. *
  http://link.springer.com/article/10.1186/s40645-015-0054-5
- "**On the Electron Dynamics During Island Coalescences in Asymmetric Magnetic Reconnection**," E. Cazzola, M. Innocenti, S. Markdis, M. Goldman, D. Newman, G. Lapenta, Physics of Plasmas, vol. 22, no. 9, September 2, 2015. *
  http://scitation.aip.org/content/aip/journal/pop/22/9/10.1063/1.4929847
- "**Particle Acceleration at Low Coronal Compression Regions and Shocks**," N. Schwadron, et al., The Astrophysical Journal, vol. 810, no. 2, September 3, 2015. *
  http://iopscience.iop.org/article/10.1088/0004-637X/810/2/97
- "**Land Cover Fraction Estimation with Global Endmembers Using Collaborative SUnSAL**," U. Kumar, et al., SPIE Proceedings, vol. 9610, Remote Sensing and Modeling of Ecosystems for Sustainability XII, September 4, 2015. *
  http://proceedings.spiedigitallibrary.org/proceeding.aspx?articleid=2436871

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

Papers (cont.)

- "**Global Coupled Sea Ice-Ocean State Estimation**," I. Fenty, D. Menemenlis, H. Zhang, Climate Dynamics (Springer), September 5, 2015. *
  http://link.springer.com/article/10.1007/s00382-015-2796-6
- "**Gas Inflow and Metallicity Drops in Star-Forming Galaxies**," D. Ceverino, et al., arXiv:1509.02051 [astro-ph.GA], September 7, 2015. *
  http://arxiv.org/abs/1509.02051
- "**Three-Dimensional Simulations of Super-Critical Black Hole Accretion Disks – Luminosities, Photon Trapping, and Variability**," A. Sadowski, R. Narayan, arXiv:1509.03168 [astro-ph.HE], September 10, 2015. *
  http://arxiv.org/abs/1509.03168
- "**A Validated Nonlinear Kelvin-Helmholtz Benchmark for Numerical Hydrodynmics**," D. Lecoanet, et al., arXiv:1509.03630 [astro-ph.IM], September 11, 2015. *
  http://arxiv.org/abs/1509.03630
- "**DeepSat—A Learning Framework for Satellite Imagery**," S. Basu, et al., arXiv:1509.03602 [cs.CV], September 14, 2015. *
  http://arxiv.org/abs/1509.03602
- "**The Origin of Molecular Cloud Turbulence**," P. Padoan, L. Pan, T. Haugboelle, A. Nordlund, arXiv:1509.04663 [astro-ph.GA], September 15, 2015. *
  http://arxiv.org/abs/1509.04663

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

Papers (cont.)

- "**Formulation and Variability of the Lofoten Basin Vortex in a High-Resolution Ocean Model**," D. Volkov, A. Kubryakov, R. Lumpkin, Deep Sea Research Part 1: Oceanographic Research Papers, vol. 105, September 14, 2015. * *http://www.sciencedirect.com/science/article/pii/S0967063715001508*
- "**Don't Forget the Forest for the Trees: The Stellar-Mass Halo-Mass Relation in Different Environments**," S. Tonnesen, R. Cen, arXiv:1509.05039 [astro-ph.GA], September 16, 2015. * *http://arxiv.org/abs/1509.05039*
- "**Local Radiation Hydrodynamic Simulations of Massive Star Envelopes at the Iron Opacity Peak**," Y.-F. Jiang, et al., arXiv:1509.05417 [astro-ph.SR], September 17, 2015. * *http://arxiv.org/abs/1509.05417*
- "**Acceleration of Wind in Optically Thin and Thick Black Hole Accretion Disks Simulated in General Relativity**," A. Moller, A. Sadowski, arXiv:1509.06644 [astro-ph.HE], September 22, 2015. * *http://arxiv.org/abs/1509.06644*

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

Presentations

- "**Panel on US Plans for Advancing HPC: Potential Implications of the White House Executive Order and NSCI**," panelists included P. Mehrotra, Broomfield, CO, September 10, 2015.
- "**Prologue O/S**," D. Talcott, presented at the PBS Works User Group, Mountain View, CA, September 16, 2015.
- "**Hybrid-Electric and Distributed Propulsion Technologies for Large Commercial Transports: A NASA Perspective**," N. Madavan, presented at the 2015 IEEE Energy Conversion Congress and Exposition (ECCE), Montreal, Canada, September 23, 2015.
- "**Writing Custom Nagios Plugins**," J. Singh, presented at the 2015 Nagios World Conference, St. Paul, MN, September 29, 2015.

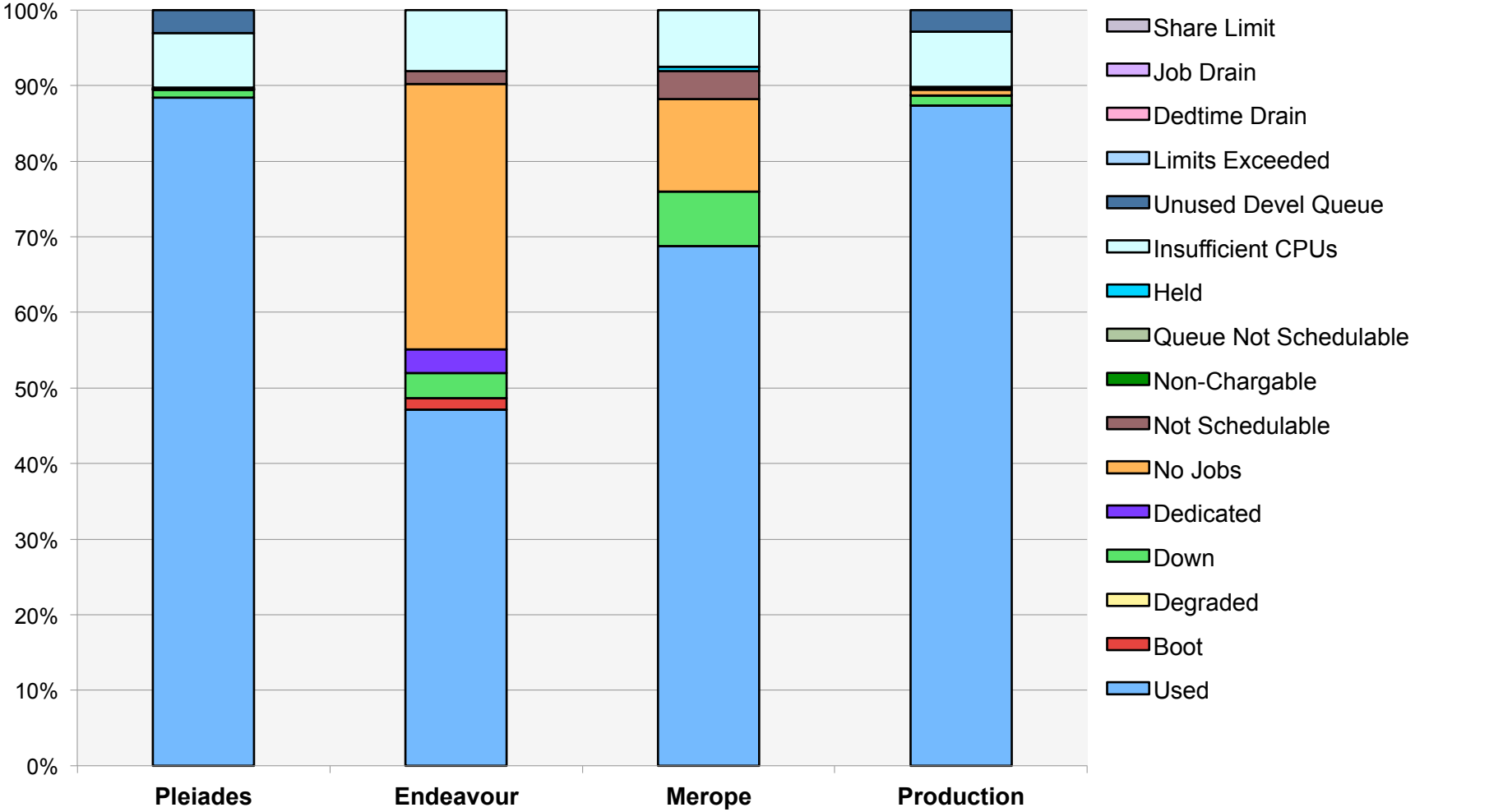
News & Events

- **IDC Hosts First Public Forum on New White House NSCI Initiative to Spur U.S. HPC Capability**, *Reuters*, September 15, 2015—International Data Corporation (IDC) held the first public panel of speakers from lead agencies—including NAS Division Chief Piyush Mehrotra, concerning the National Strategic Computing Initiative. *http://www.reuters.com/article/2015/09/15/co-idc-idUSnBw155574a+100+BSW20150915*
  - **HPC User Forum Presses NSCI Panelists on Plans**, *HPCwire*, September 17, 2015. *http://www.hpcwire.com/2015/09/17/hpc-user-forum-presses-nsci-panelists-on-plans/*
  - **User Agency Panel Discussion on NSCI Initiative**, *insideHPC*, September 21, 2015. *http://insidehpc.com/2015/09/user-agency-panel-discussion-on-the-nsci-initiative/*
- **Deep Belief in Networks at the Heart of NASA Image Classification**, *The Platform*, September 21, 2015—A team from the NASA Advanced Supercomputing Division have sought a new blend of deep learning techniques that can build on existing neural nets to create something robust enough for satellite datasets. *http://www.theplatform.net/2015/09/21/deep-belief-networks-at-heart-of-nasa-image-classification/*

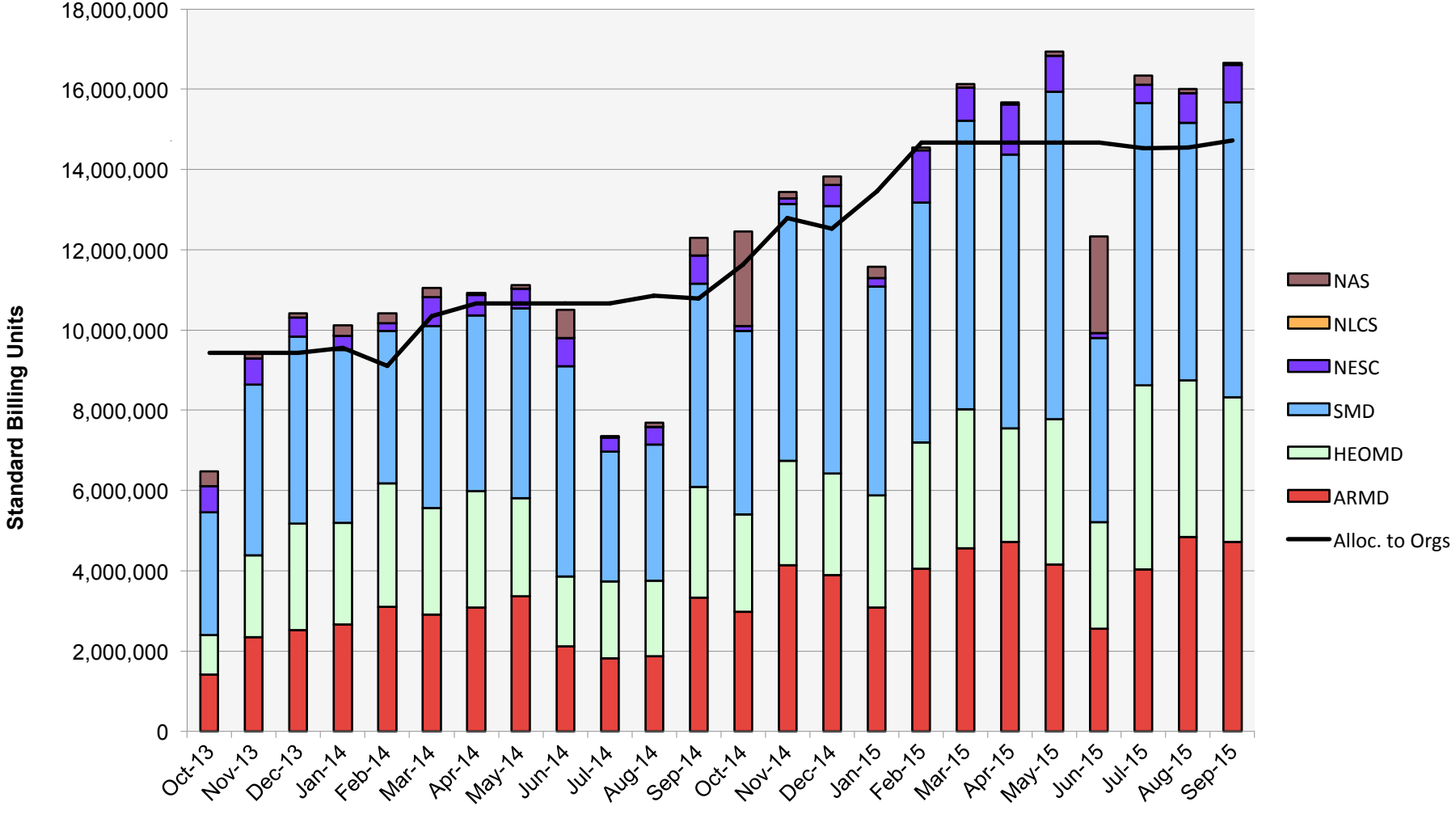
News & Events (cont.)

- **D-Wave Systems Announces Multi-Year Agreement to Provide Its Technology to Google, NASA, and USRA's Quantum Artificial Intelligence Lab**, *D-Wave press release*, September 28, 2015—D-Wave announces a new agreement with USRA and Google covering the installation of a succession of D-Wave systems at the NASA Advanced Supercomputing facility.
  http://www.dwavesys.com/press-releases/d-wave-systems-announces-multi-year-agreement-provide-its-technology-google-nasa-and
  - **D-Wave Systems Announces Agreement to Provide Technology to Google, NASA, and USRA**, *HPCwire*, September 28, 2015.
    http://www.hpcwire.com/off-the-wire/d-wave-systems-announces-agreement-to-provide-technology-to-google-nasa-and-usra/

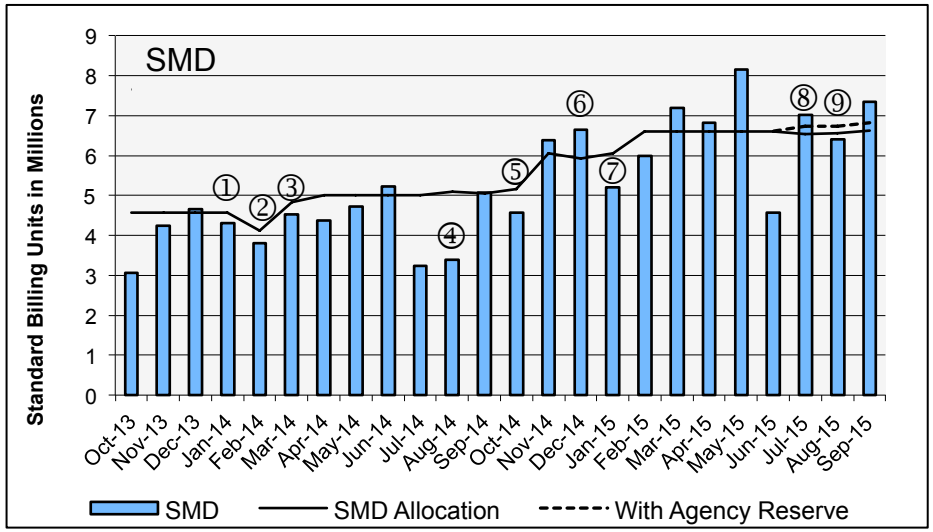
HECC Utilization

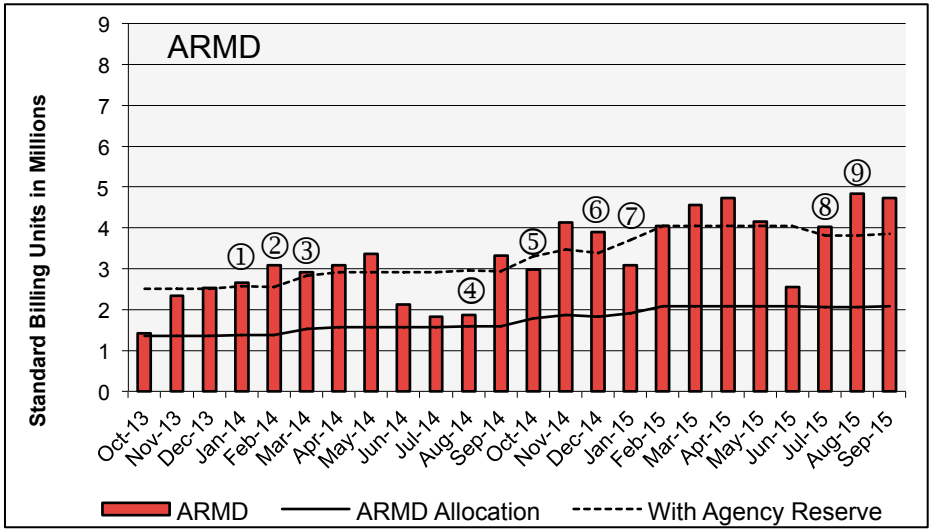


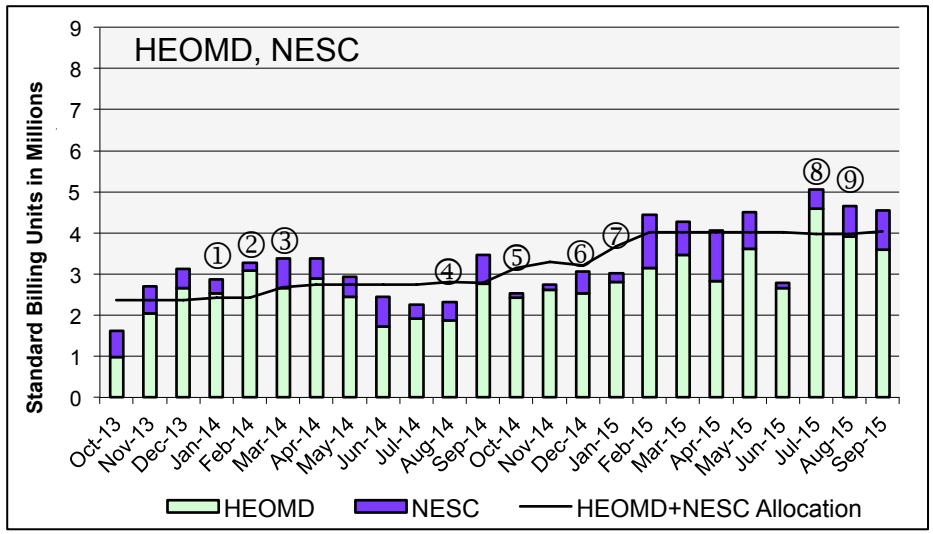
HECC Utilization Normalized to 30-Day Month



HECC Utilization Normalized to 30-Day Month







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

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

③ 4 Ivy Bridge Racks added mid-March

④ 6 Westmere Racks added to Merope, Merope Harpertown retired

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

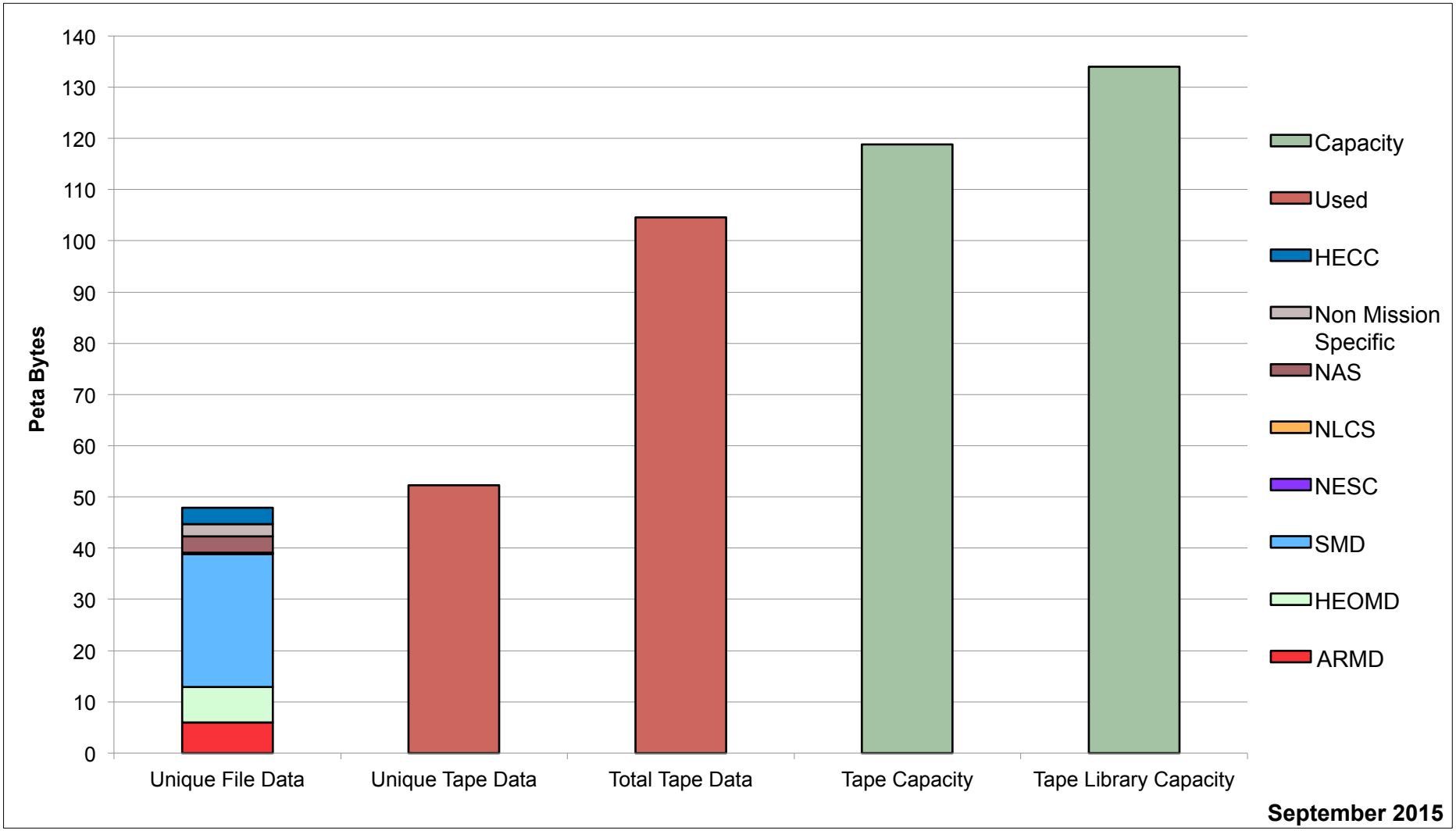
⑥ 16 Westmere Racks retired

⑦ 14 Haswell racks added

⑧ 7 Merope Nehalem Racks removed

⑨ 7 Merope Westmere Racks added

Tape Archive Status



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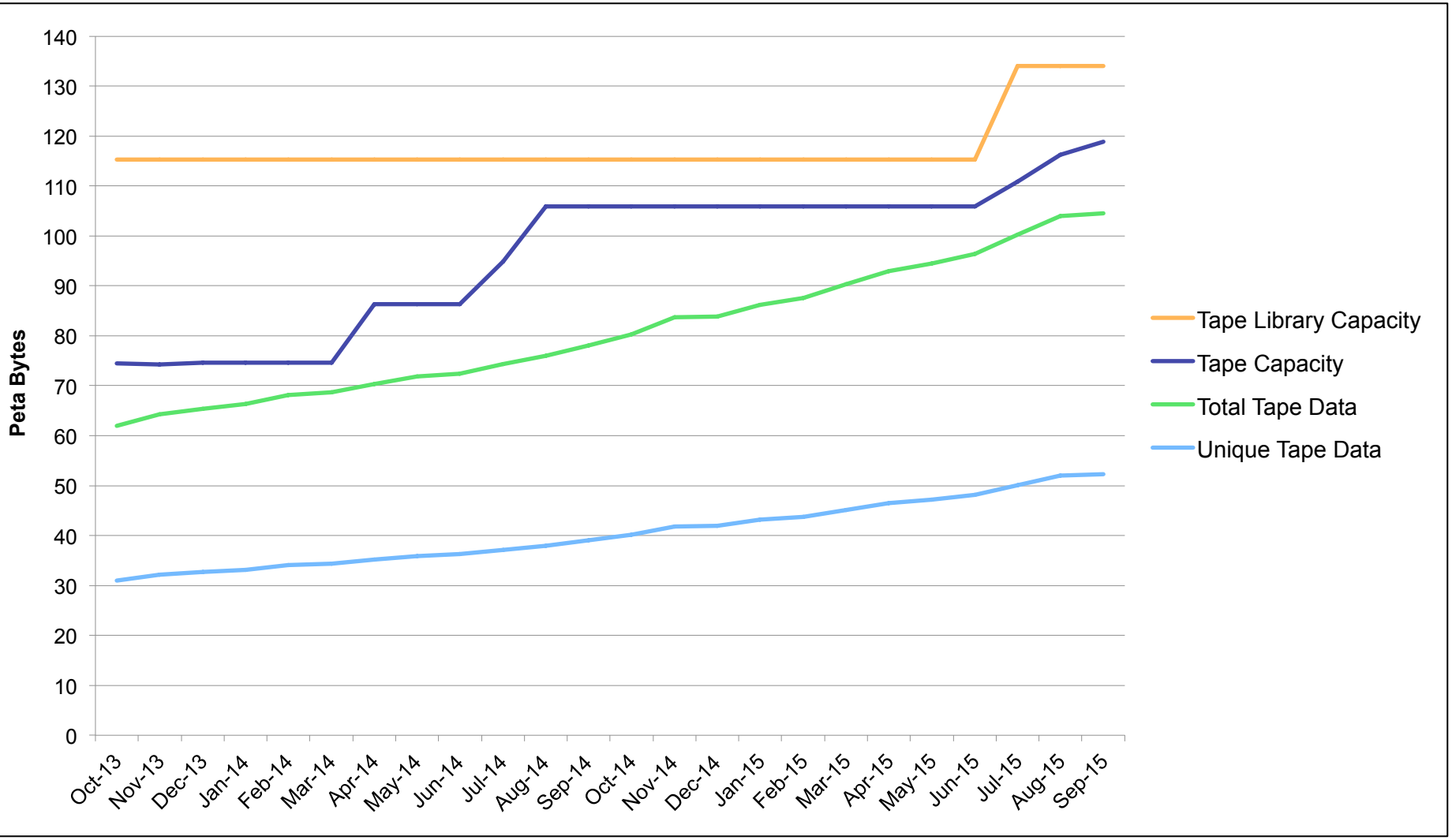
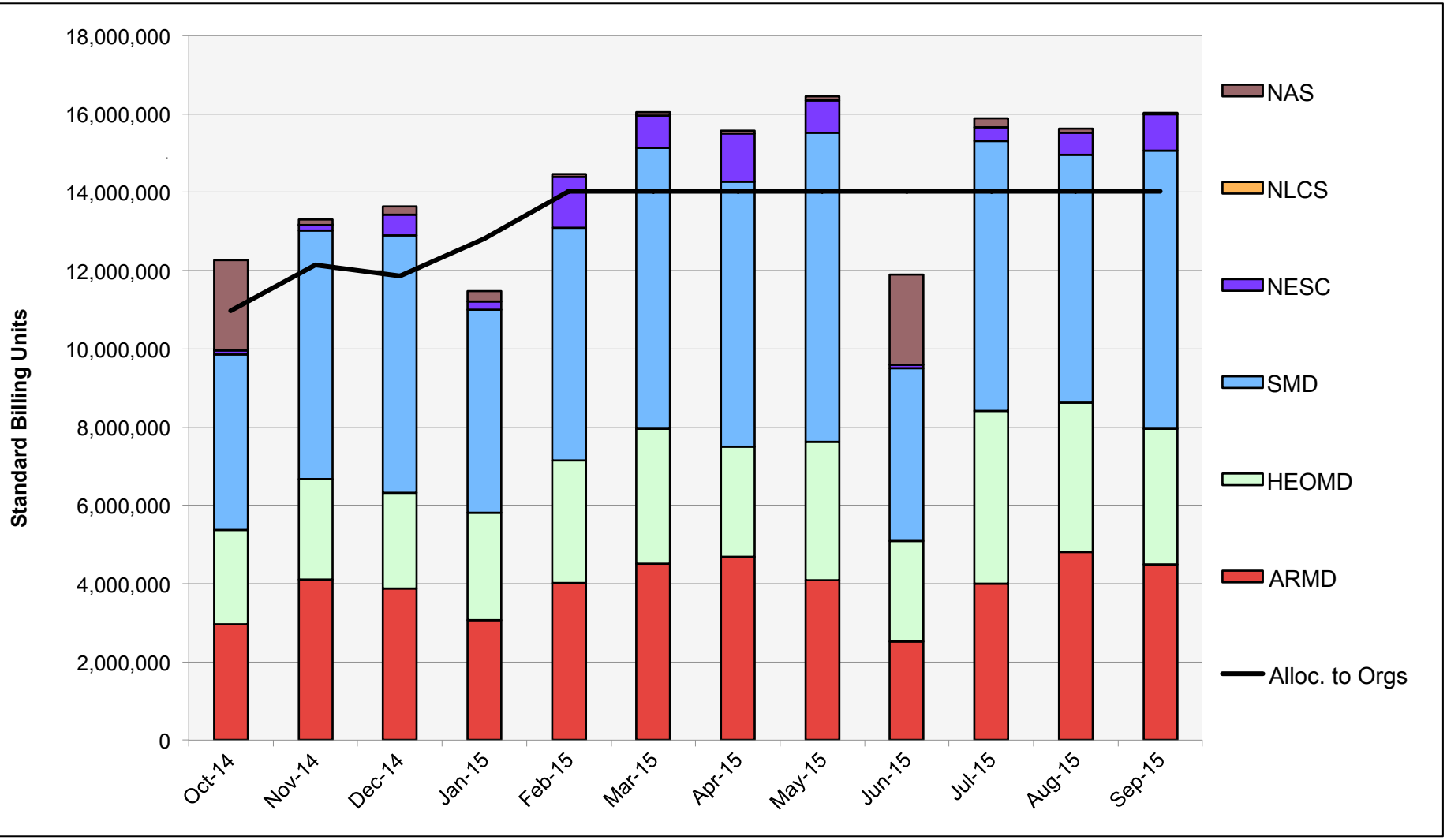
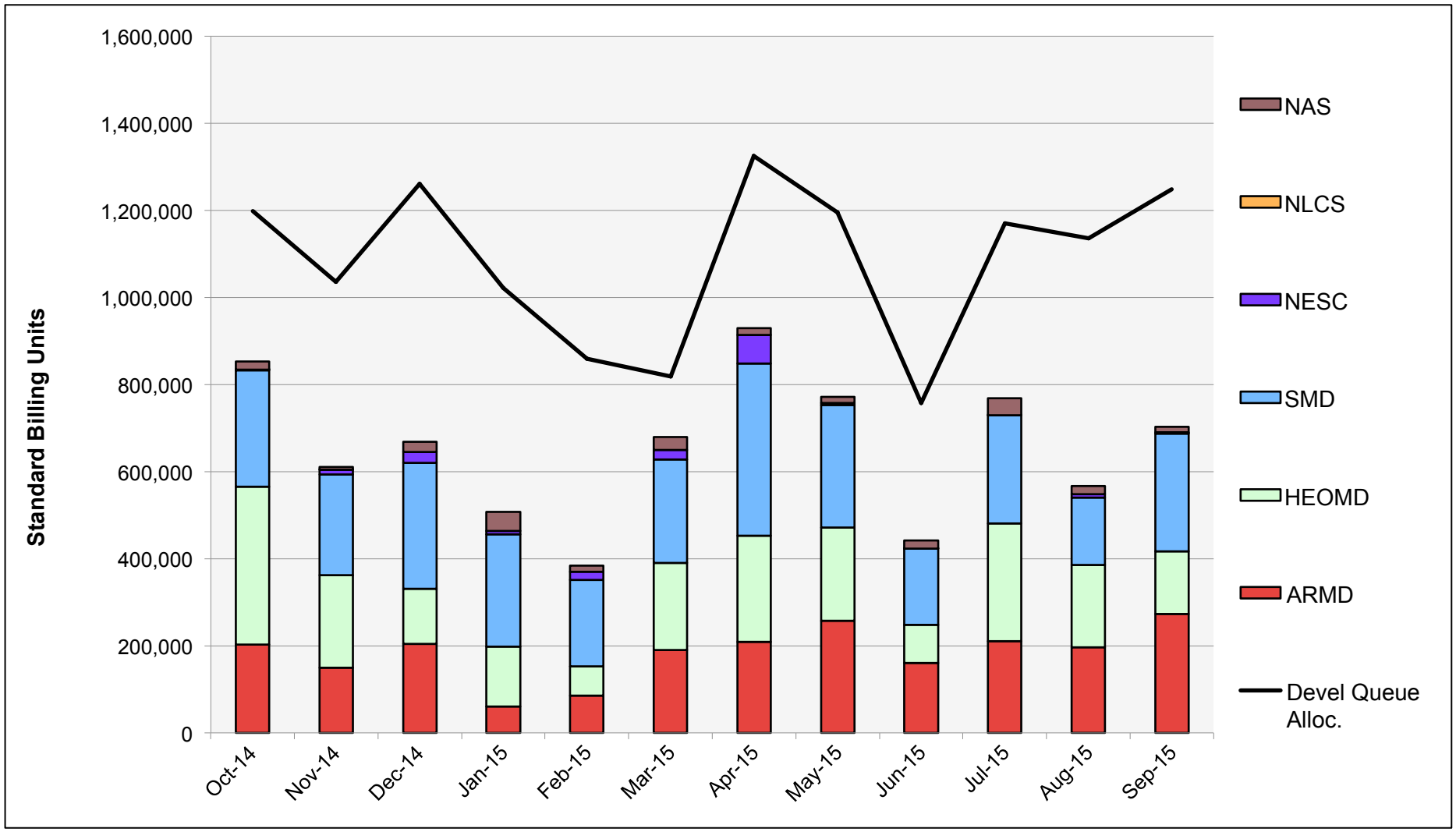


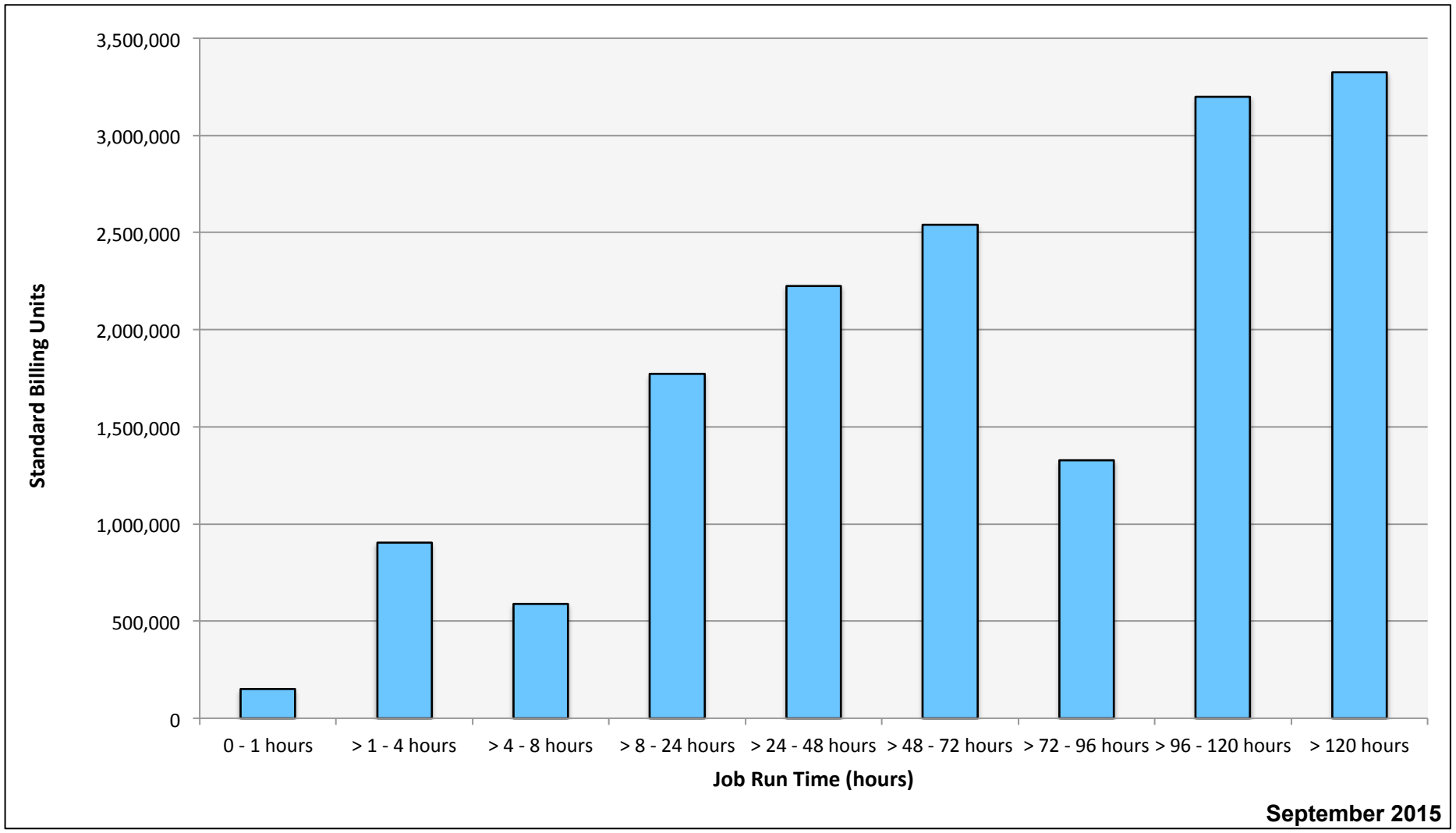
Pleiades:
SBUs Reported, Normalized to 30-Day Month



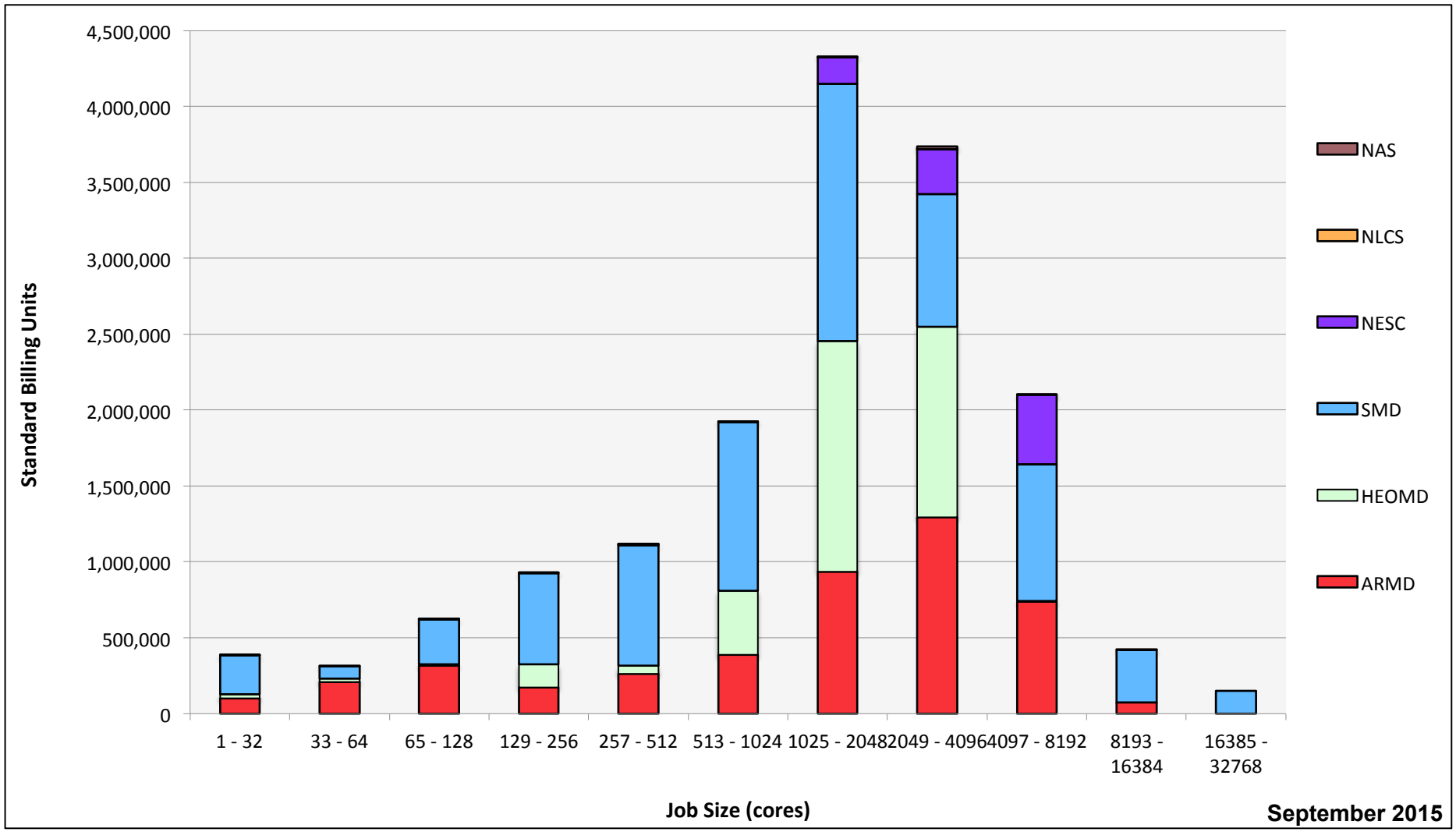
Pleiades:
Devel Queue Utilization



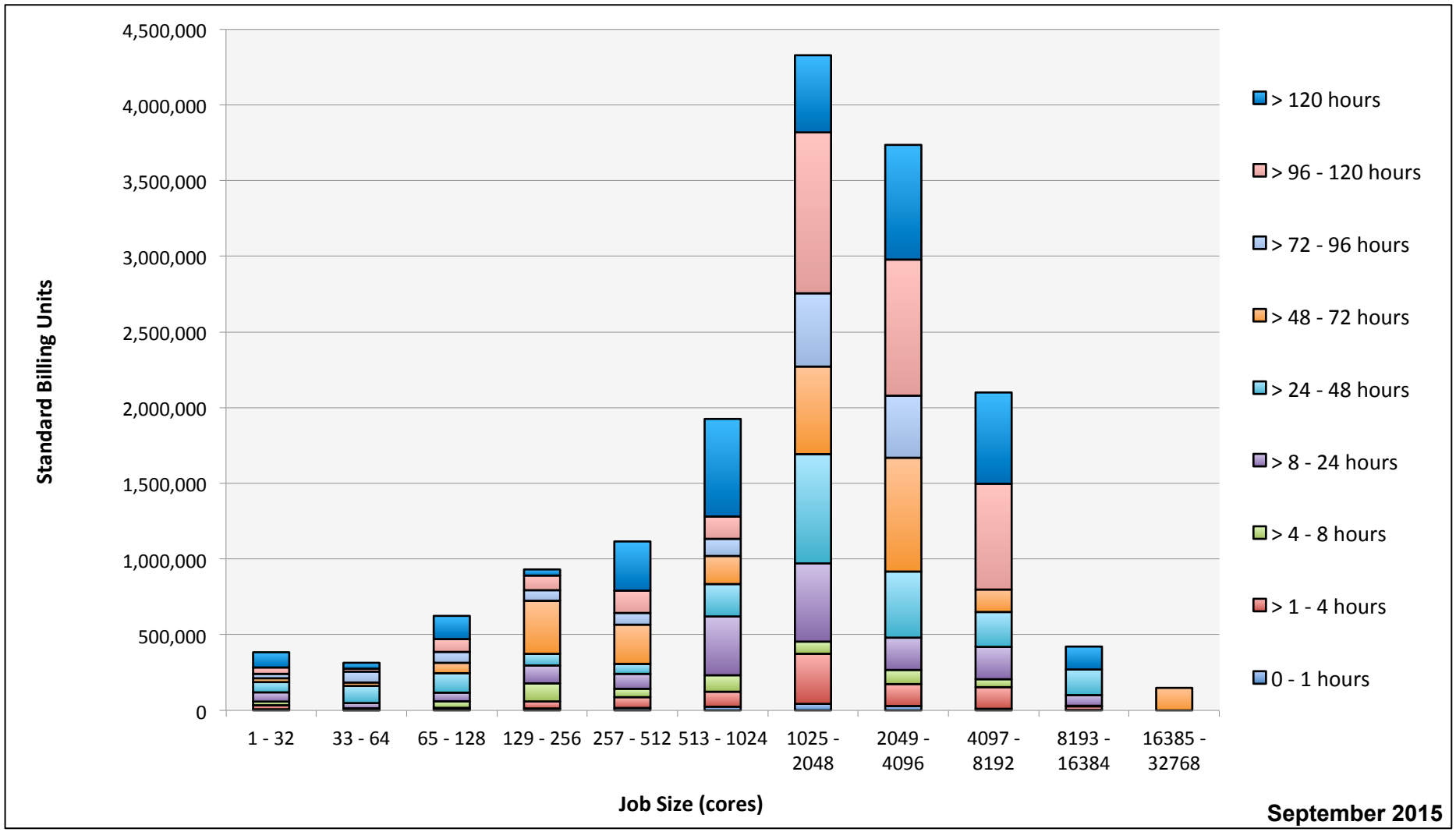
Pleiades:
Monthly Utilization by Job Length



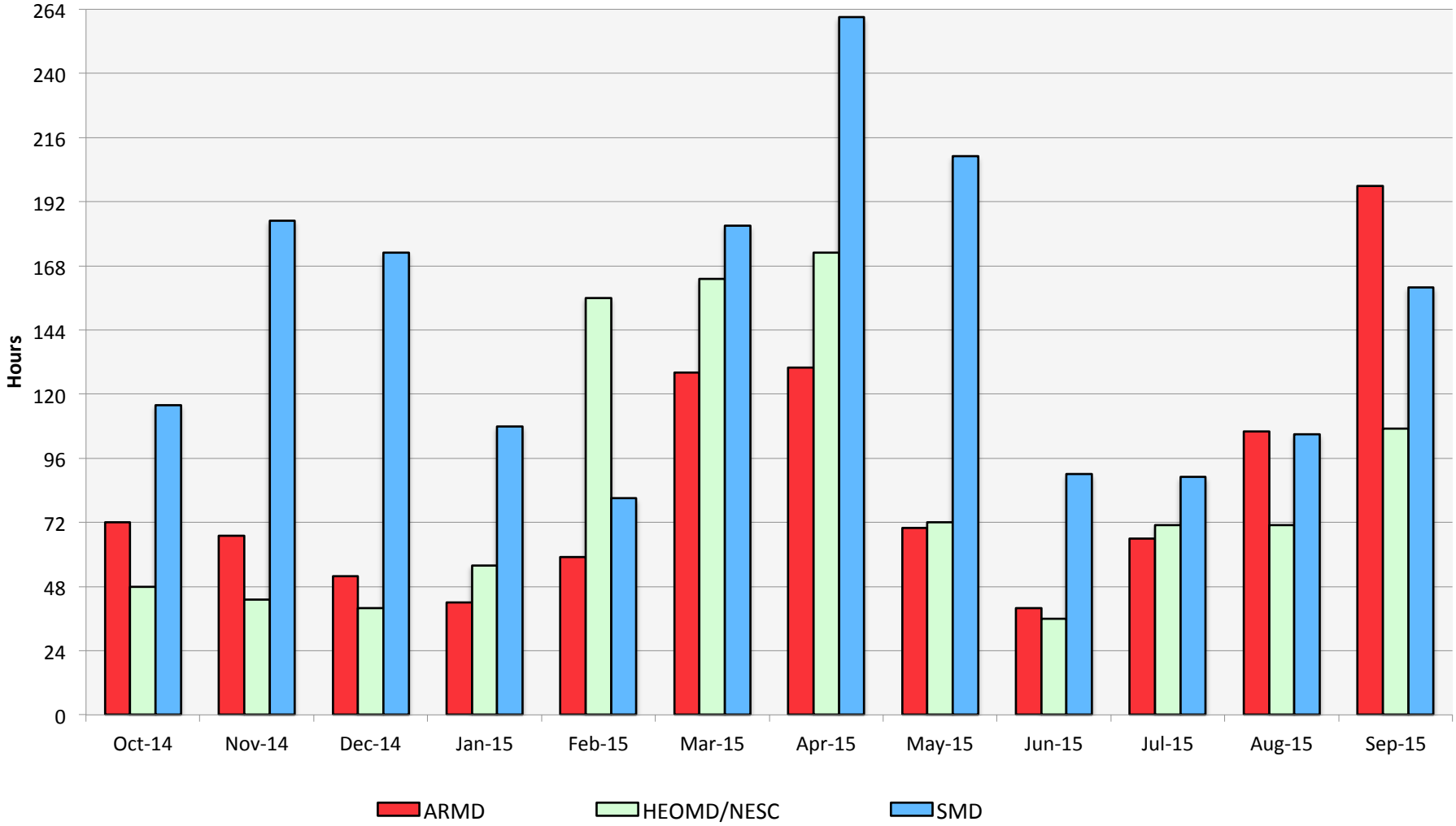
Pleiades:
Monthly Utilization by Size and Mission



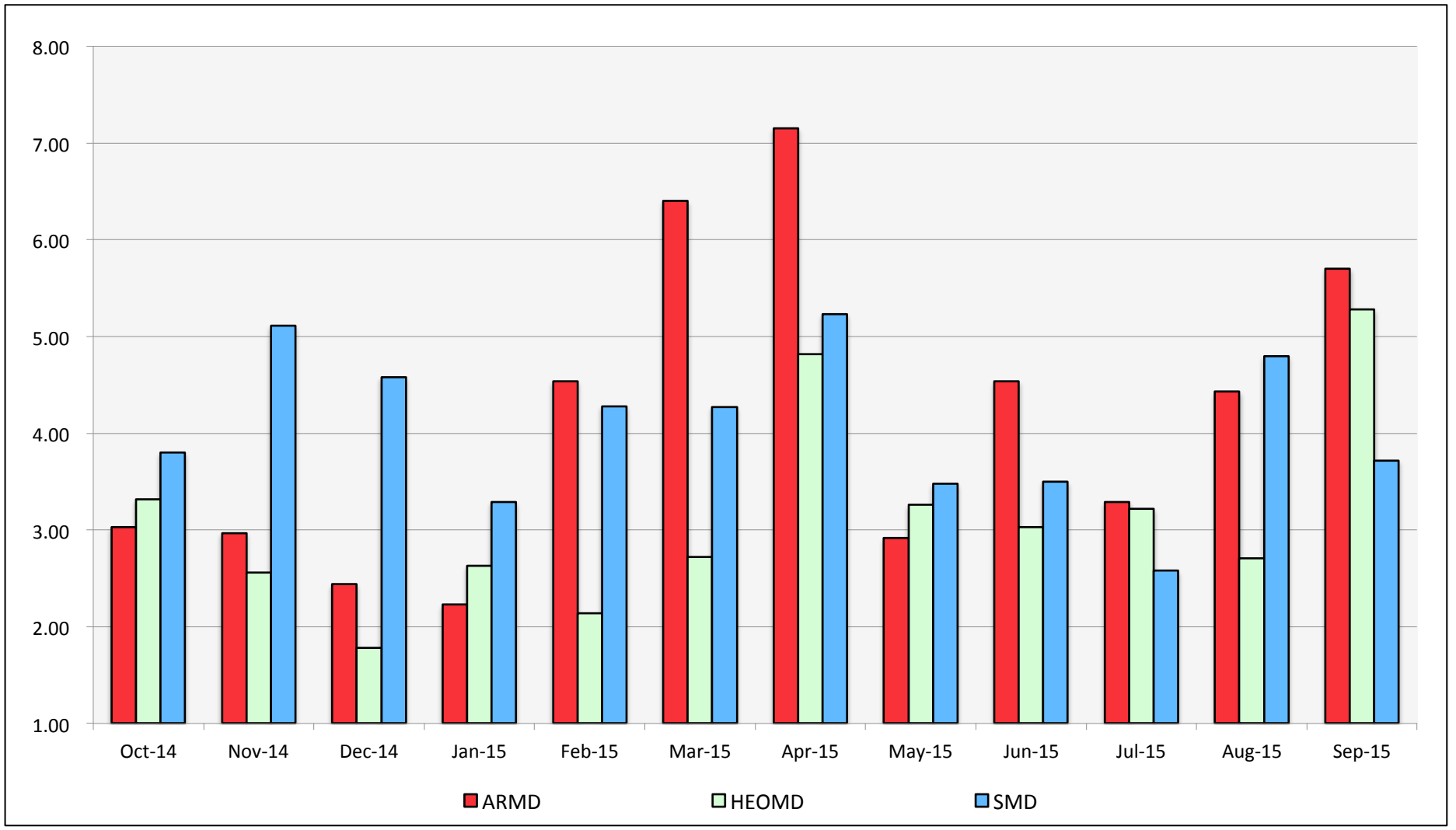
Pleiades:
Monthly Utilization by Size and Length



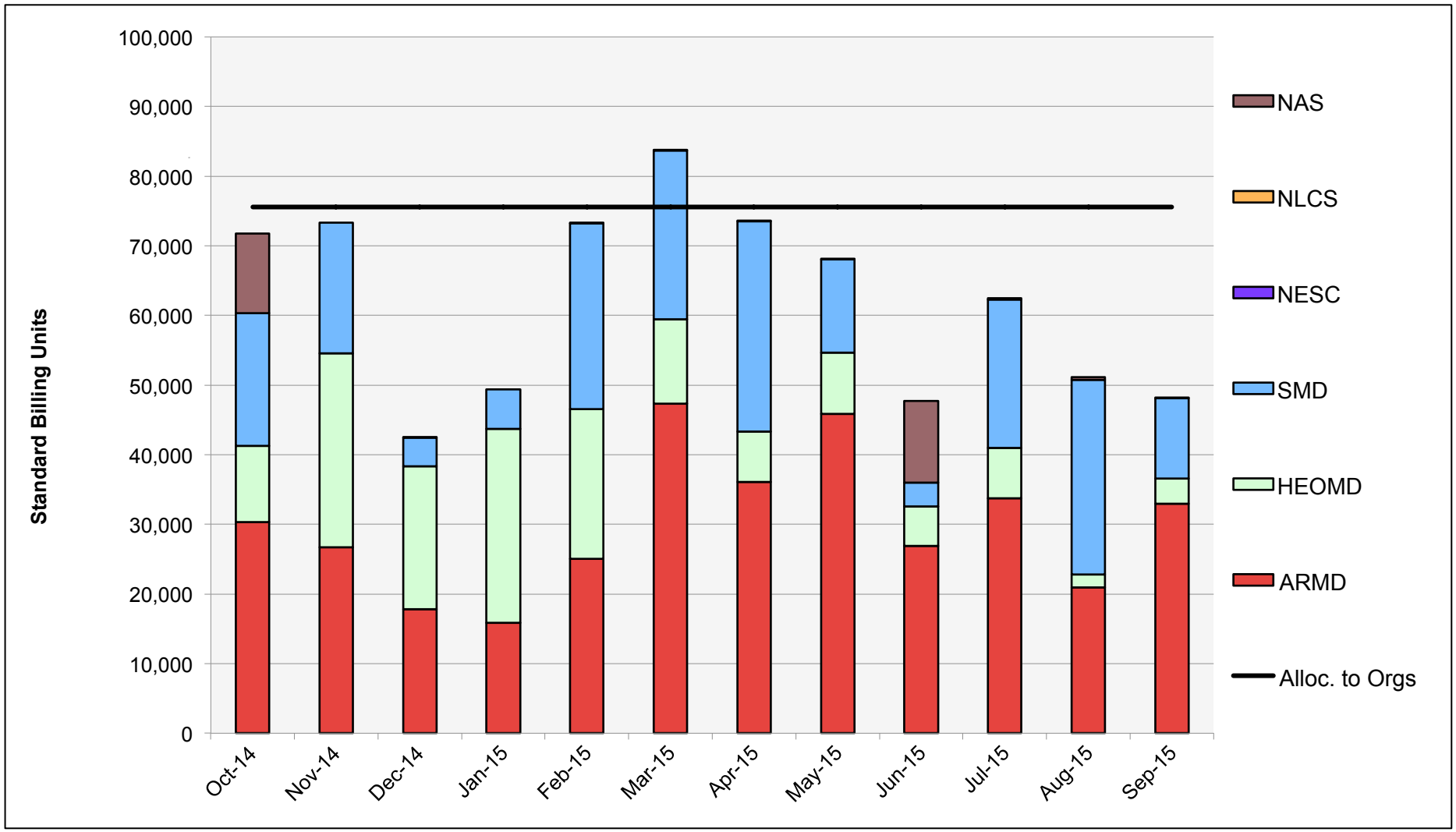
Pleiades:
Average Time to Clear All Jobs



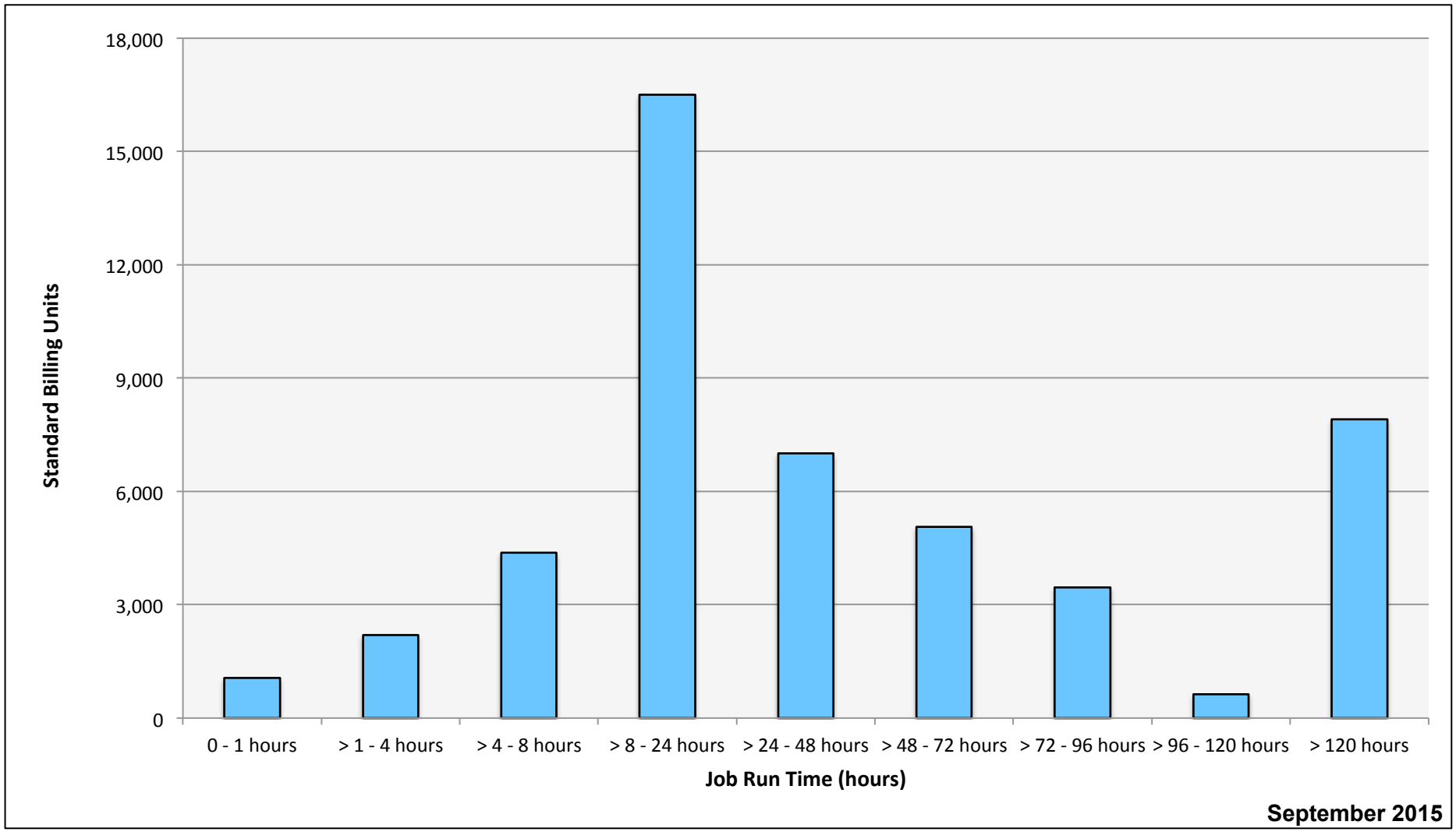
Pleiades:
Average Expansion Factor



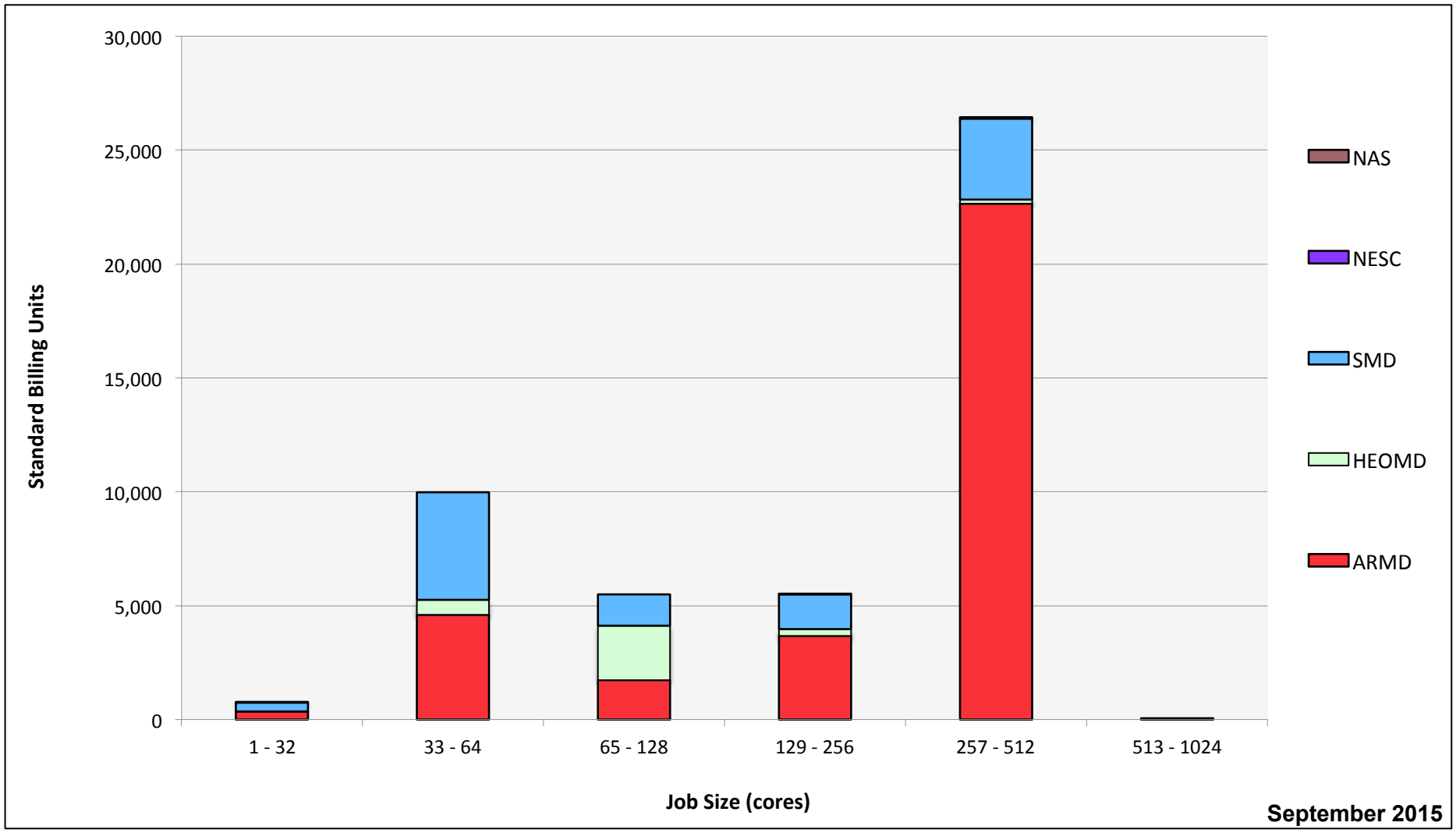
Endeavour:
SBUs Reported, Normalized to 30-Day Month



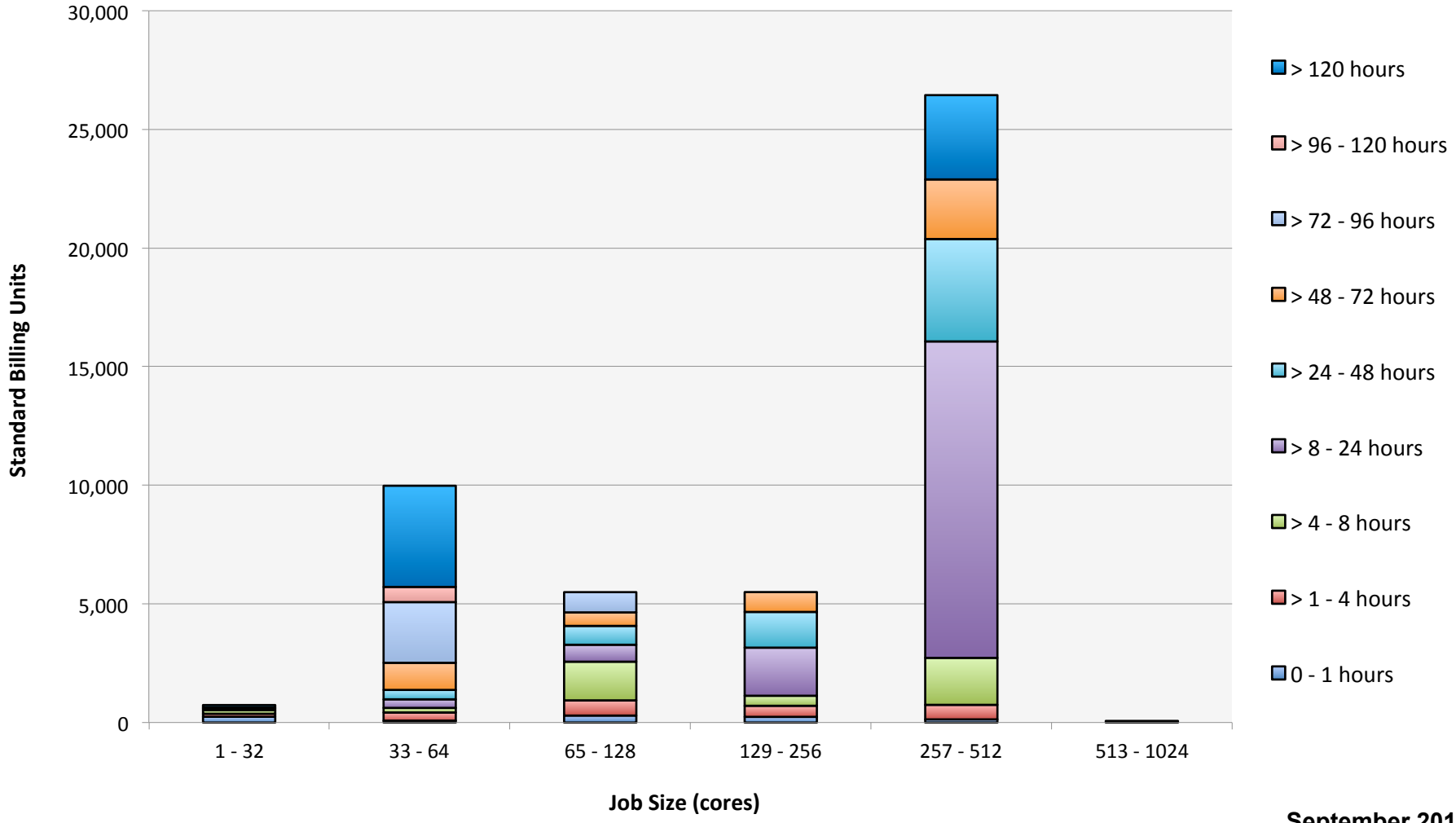
Endeavour:
Monthly Utilization by Job Length



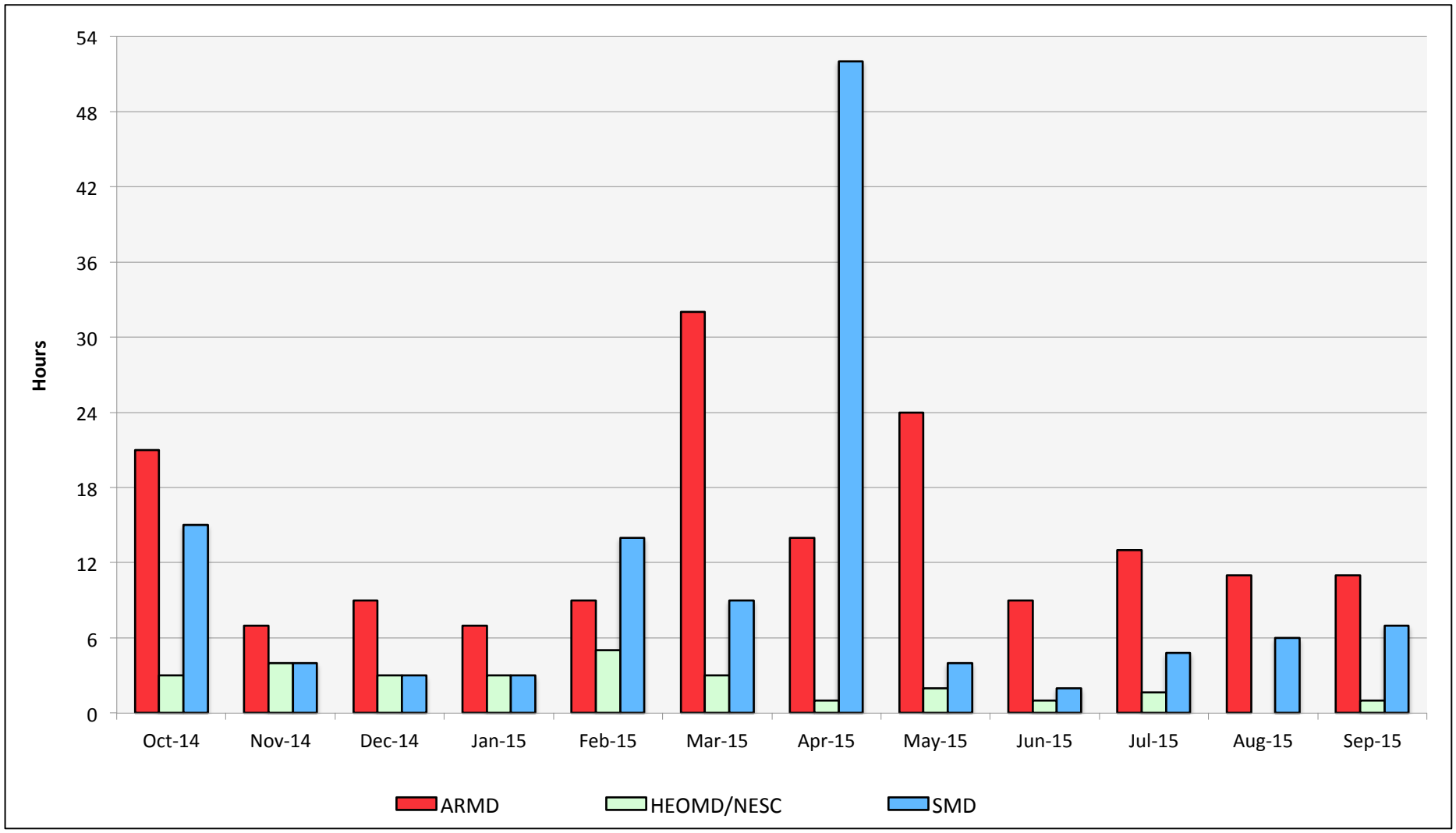
Endeavour:
Monthly Utilization by Size and Mission



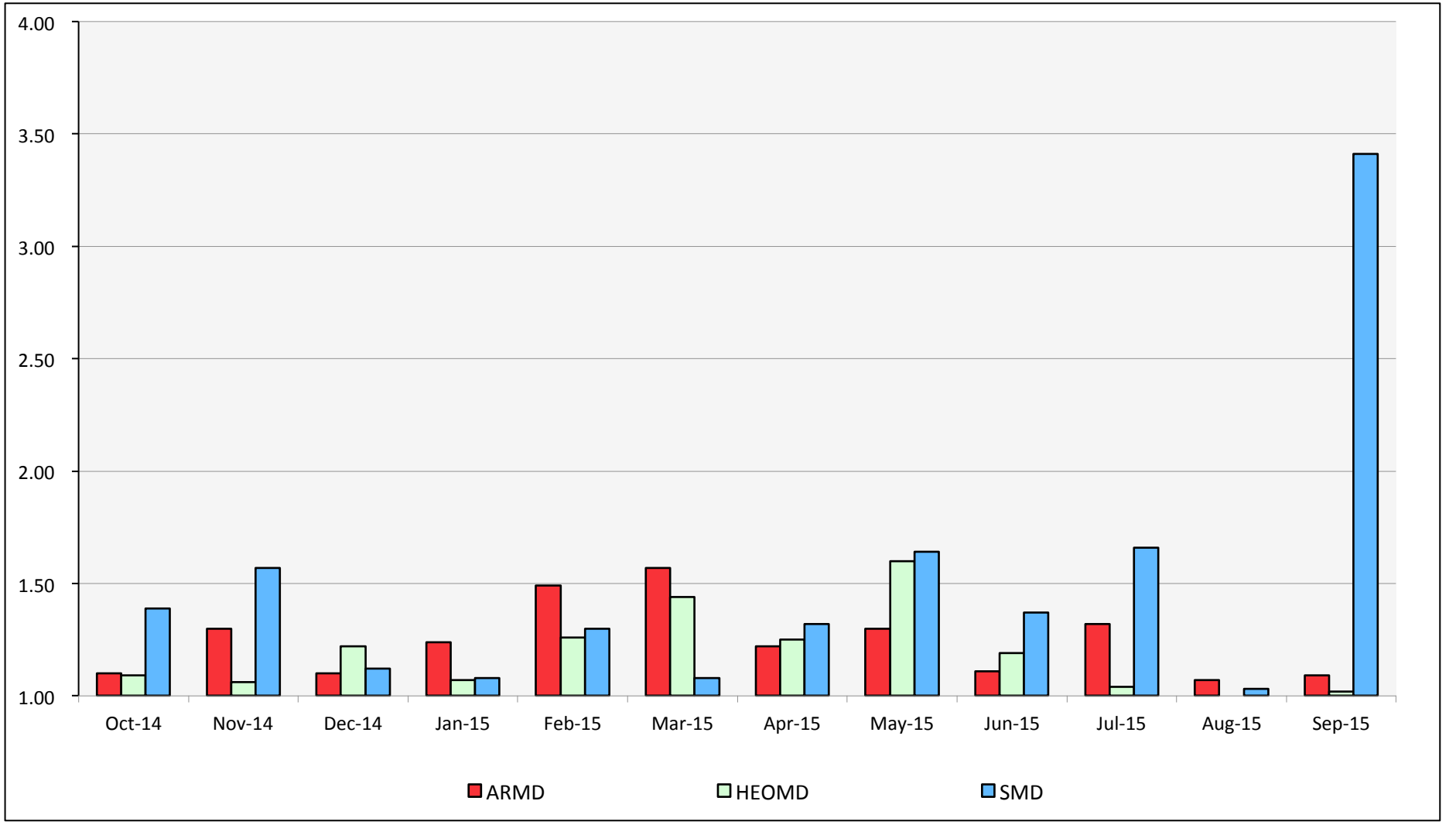
Endeavour:
Monthly Utilization by Size and Length



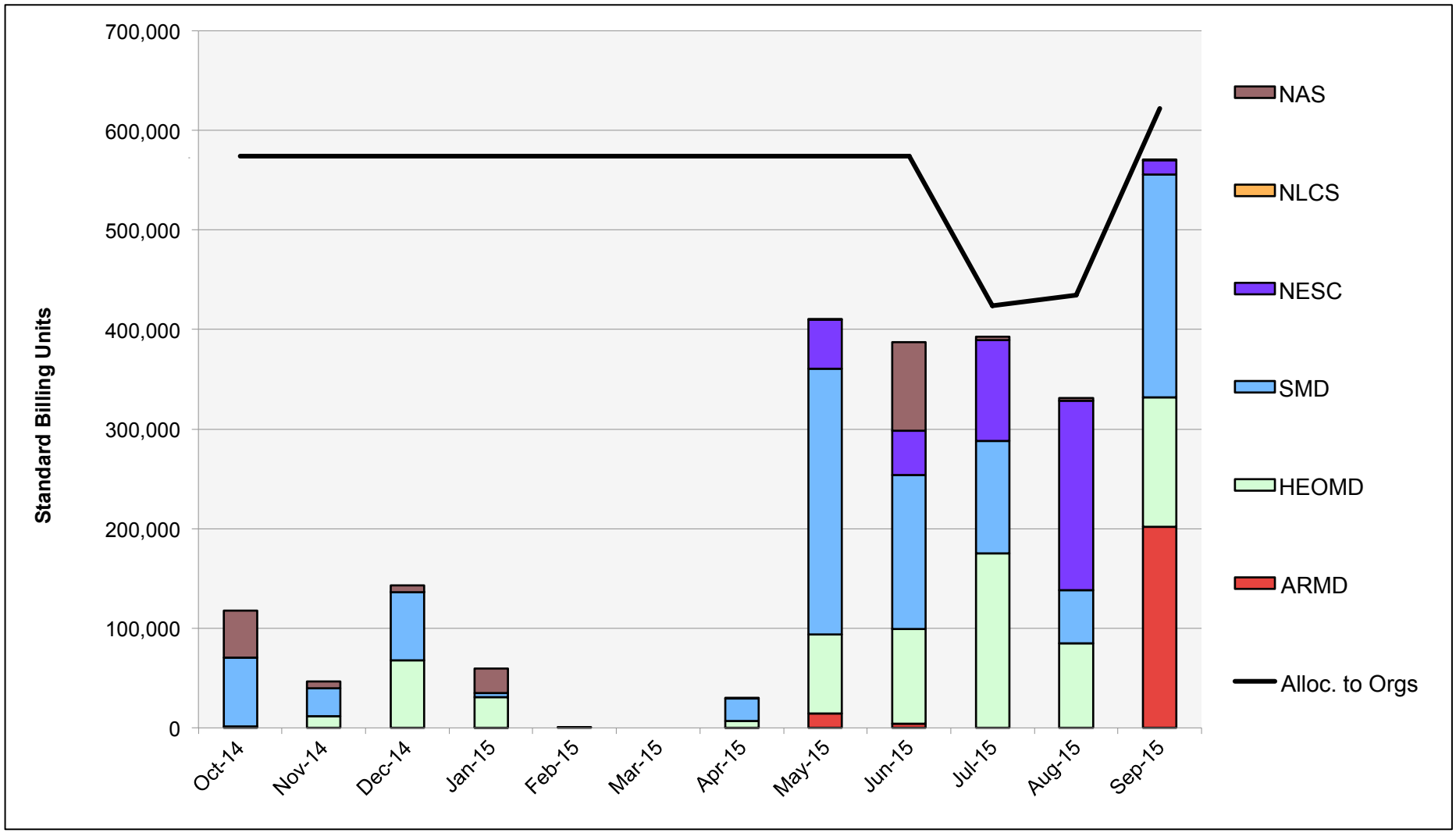
Endeavour:
Average Time to Clear All Jobs



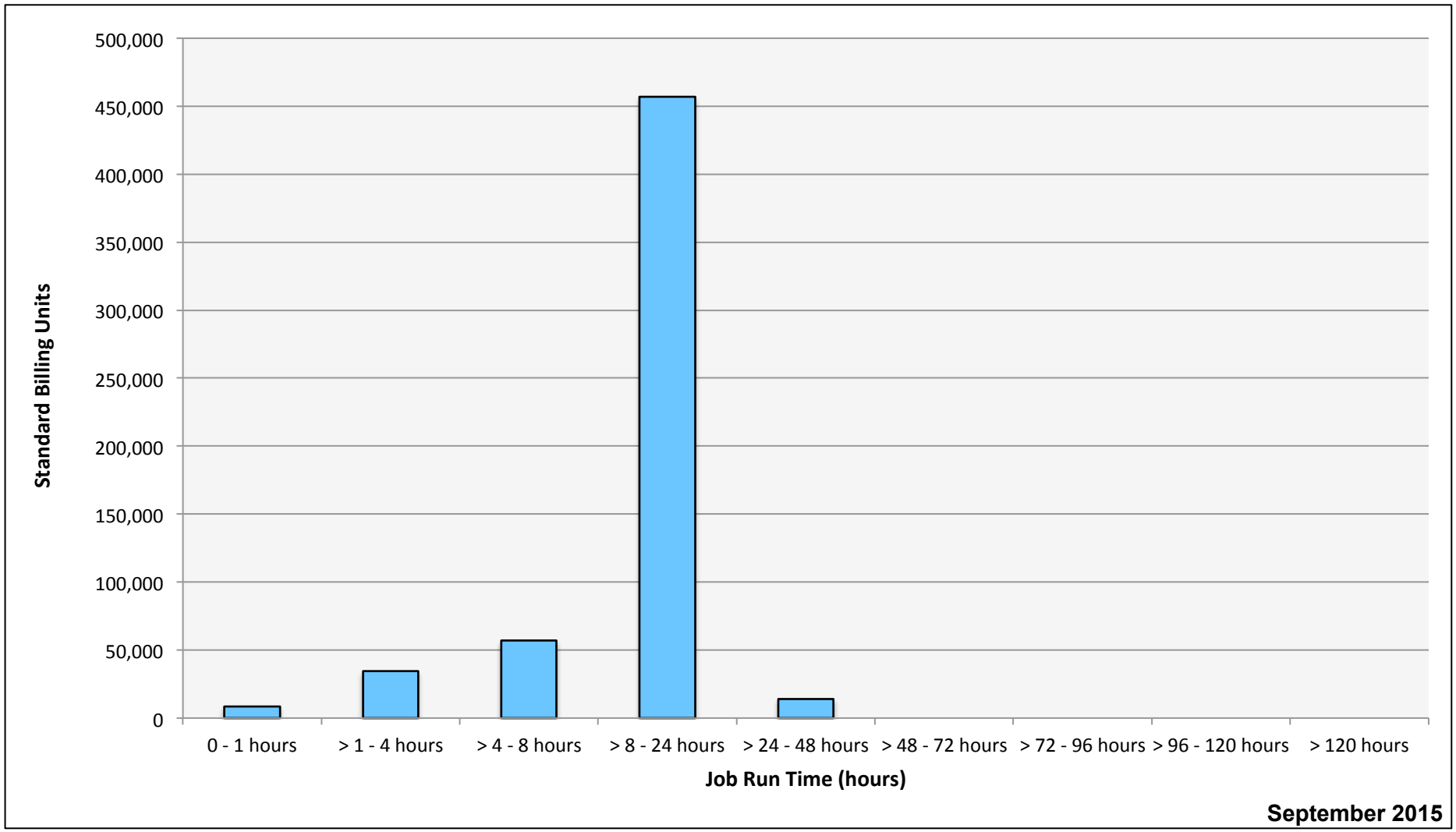
Endeavour:
Average Expansion Factor



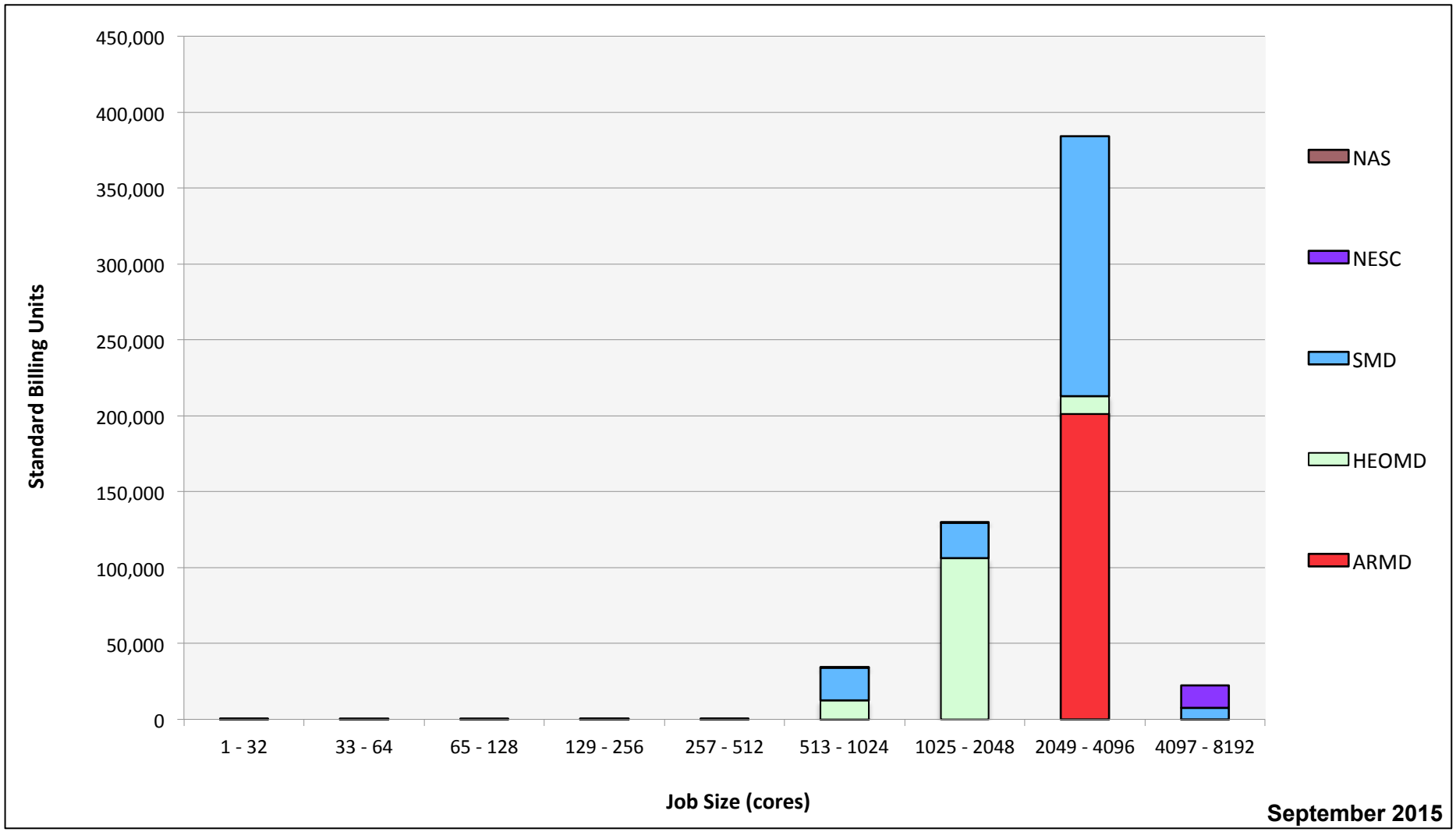
Merope:
SBUs Reported, Normalized to 30-Day Month



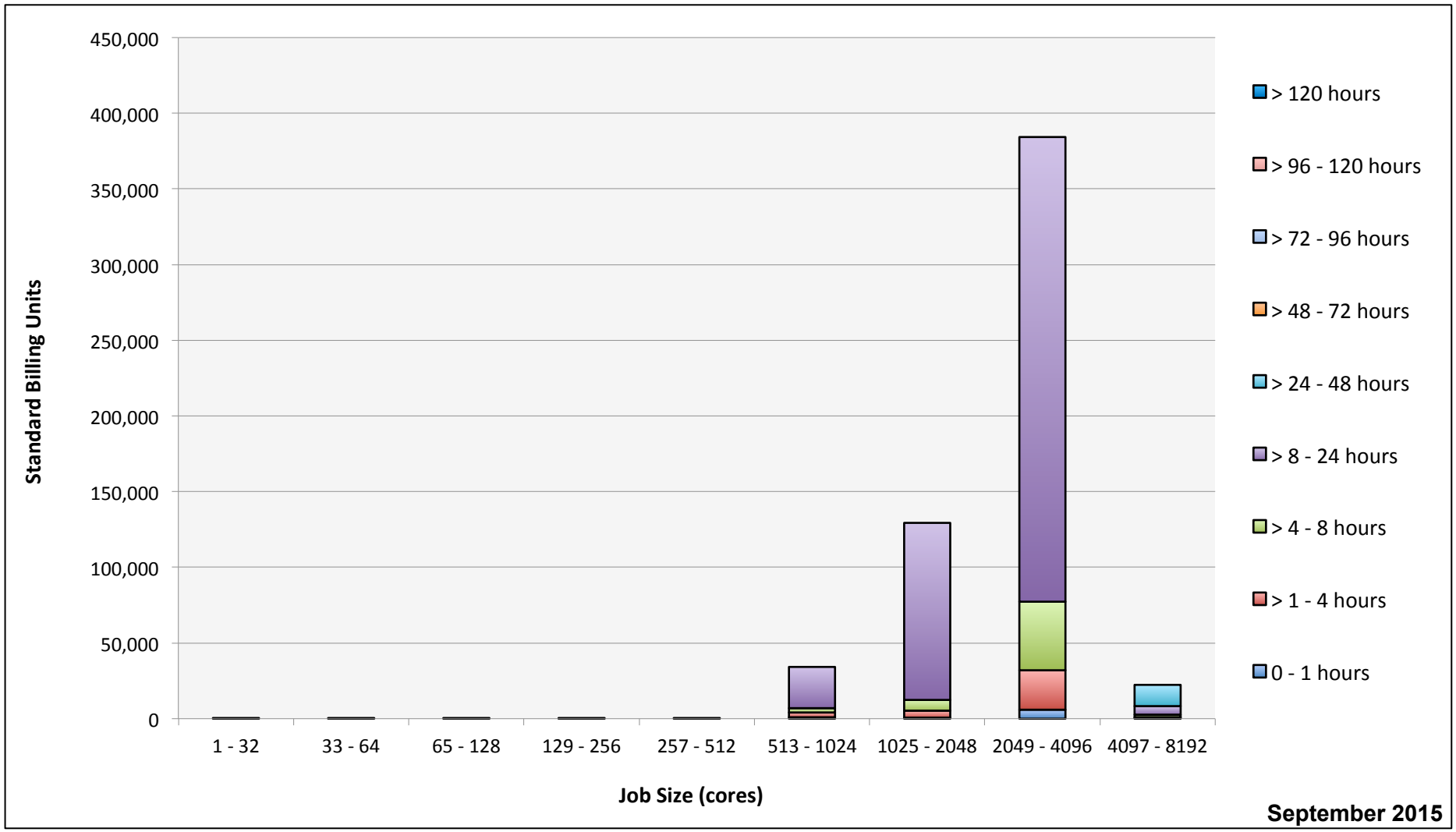
Merope:
Monthly Utilization by Job Length



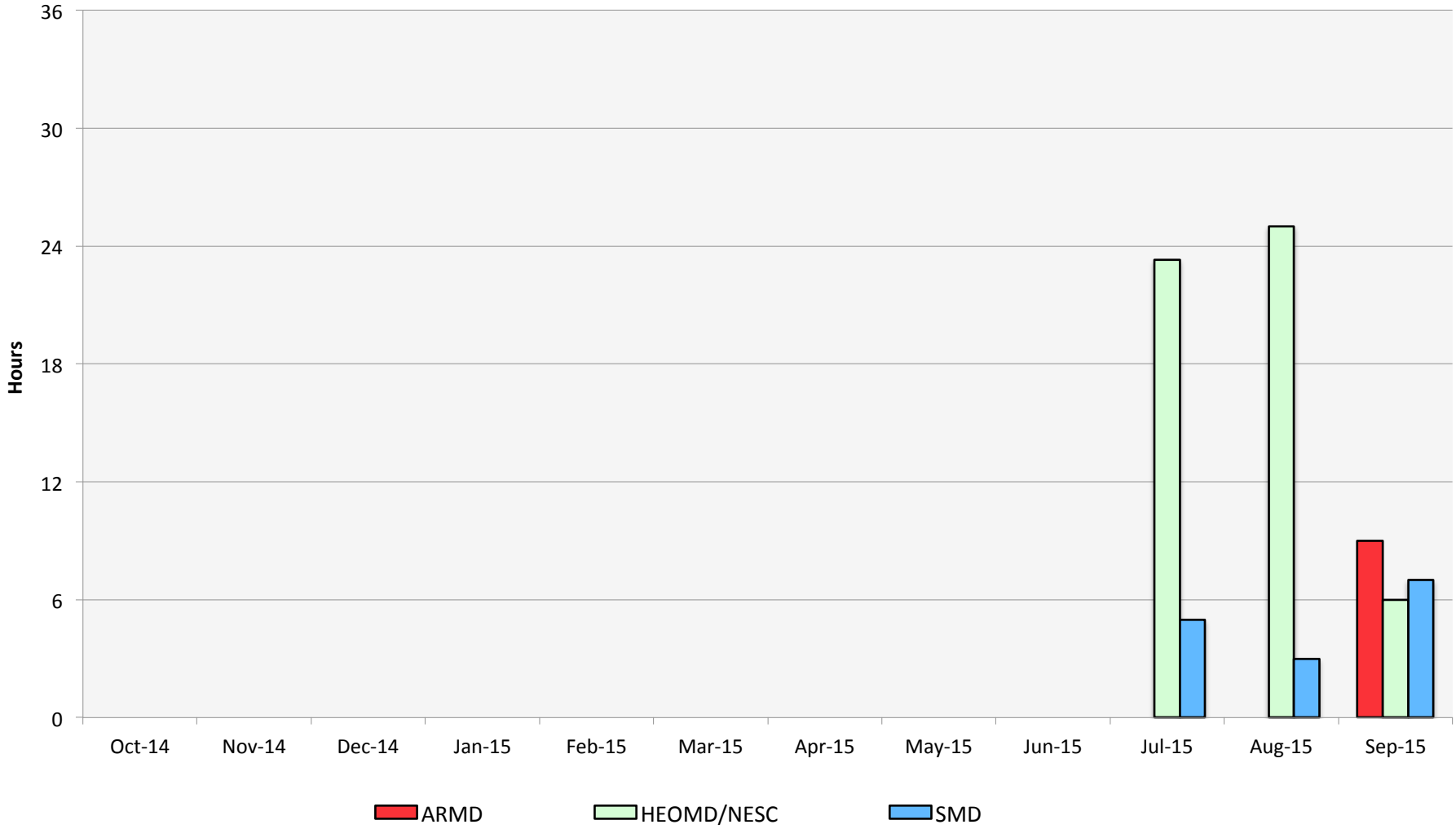
Merope:
Monthly Utilization by Size and Mission



Merope:
Monthly Utilization by Size and Length



Merope:
Average Time to Clear All Jobs



Merope:
Average Expansion Factor