Project Status Report

High End Computing Capability
Strategic Capabilities Assets Program

August 10, 2016

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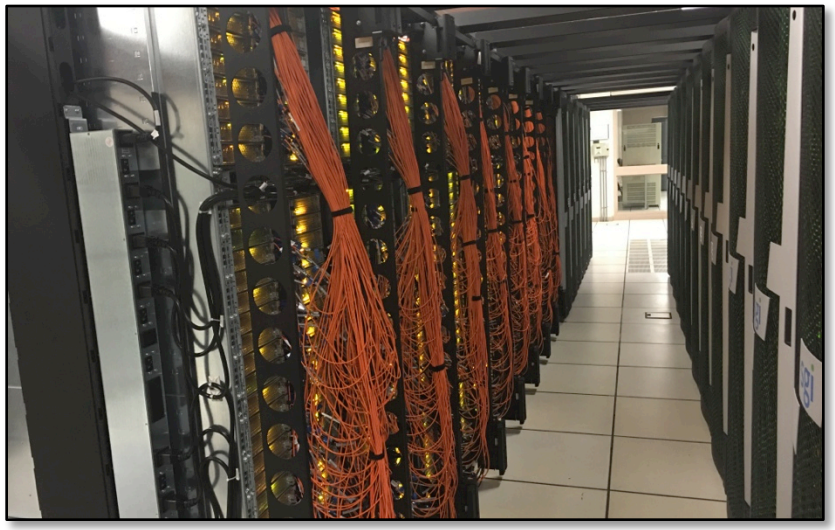
Pleiades Augmented with Broadwell Processors to Increase ARMD's Allocation

- The HECC Supercomputing Systems team augmented the Pleiades supercomputer with 14 additional racks of the latest-generation Intel E5-2680v4 (Broadwell) processors. This expanded the system's total peak performance from 6.28 petaflops (PF) to 7.24 PF. Of the 14 racks, 10.5 were procured for ARMD, adding 75% to their baseline allocation.
- HECC and SGI engineers completed system installation, configuration, testing, and release into production in 8 calendar days – 8 days ahead of schedule. The accelerated release into production provided an additional 780,000 SBUs to users.
- HECC engineers integrated the Broadwell racks into the Pleiades InfiniBand fabric using an in-house developed live-integration method to minimize the impact on production compute cycles for users.
- In order for the Broadwell racks to be deployed, all of the Pleiades Westmere racks were retired due to power and cooling constraints in the primary compute facility (N258). Only 3.5 Broadwell racks were required to provide the equivalent processing power of the retired Westmere racks.

Mission Impact: To meet NASA's rapidly increasing requirements for high-performance computing, HECC must regularly and significantly upgrade and replace the supercomputing resources provided to the agency.



The addition of 14 Broadwell racks increased the Pleiades supercomputer's peak performance by 15 percent—from 6.28 to 7.24 petaflops.

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 Augments Lustre Short-Term Storage Capacity

- The HECC Supercomputing Systems team expanded the short-term Lustre disk storage available for HECC users with repurposed storage hardware.
- A total of 1.4 petabytes (PB) of storage was added transparently to users actively utilizing the filesystems. The storage increase was split between two existing filesystems, nobackupp6 and nobackupp9.
- The storage subsystem was previously utilized by the HECC Visualization team, but with a new storage system available for them, some resources were reallocated for use by the general HECC community.
- A portion of the retired storage subsystem was retained as on-site spare parts to minimize the maintenance costs of the storage subsystem.

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.

The Lustre *nobackup* filesystems are the primary systems used for temporary storage. The storage capacity on two combined filesystems increased by 25% with an upgrade in July 2016.

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

"Self Service" Application Promotes Ease in Patching NAS Macs and Improves Security

- Patching mobile systems has historically been time consuming while waiting for users to put their systems on the network. To reduce the time it takes to patch HECC/NAS Macs, the Engineering Servers and Services (ESS) team developed the "Self Service" application, allowing users to patch their own systems at their convenience.
- ESS defines patching policies in Casper, and the Self Service application allows users to trigger these policies for installation. By using Self Service, users can initiate important updates when it is least disruptive to their work.
- ESS also developed policy configurations and "smart groups" that prevent duplication of patching while ensuring that all Macs receive the updates through Self Service or an automatic push from the Casper application.
- Future enhancements will include deployment of commonly requested software and updated versions of familiar apps. Various maintenance tasks and workarounds for common issues will also be available through the app.

Mission Impact: The HECC-developed Self Service application promotes ease in patching of mobile systems, thus reducing security vulnerabilities in the HECC/NAS systems.

The HECC/NAS "Self Service" icon displays the number of patching policies available for each user's Mac.

POC: Ted Bohrer, theodore.w.bohrer@nasa.gov, (650) 604-4335, NASA Advanced Supercomputing Division, ADNET Systems

Mini Hyperwall Upgraded to New Servers Running Red Hat Linux

- To improve the usage, performance, and reliability of the mini-hyperwall used at the Supercomputing Conferences and during NAS facility tours, the Engineering Servers and Services (ESS) team upgraded the server nodes from Mac Minis to Dell mini PCs running Red Hat Linux. The team significantly improved the user interface for demonstrations, and trained presenters to ensure professional and trouble-free presentations.
- ESS worked with the Network team to define a private virtual LAN for the mini-hyperwall to securely isolate the system, but allow open ports for system patching, CFEngine support, and security scanning.
- ESS also developed new scripts to automate the demos, and tailored the workflow to the new configuration. The servers are now supported under the standard ESS support model and the NAS Security Plan.
- As a result of this new configuration, the mini-hyperwall will also be faster, more reliable, and more efficient to operate and maintain by staff supporting NASA's booth at Supercomputing conferences in the future.

Mission Impact: The upgraded mini-hyperwall provides a reliable platform for tours and demonstrations to showcase NASA science and engineering accomplishments enabled by HECC resources.

Space exploration simulations shown on the mini-hyperwall provided the perfect backdrop for NASA Deputy Administrator Dava Newman's interview with Xploration Outer Space for Fox Saturday in June 2016. HECC systems experts rebuilt the mini-hyperwall with new server nodes to improve its performance.

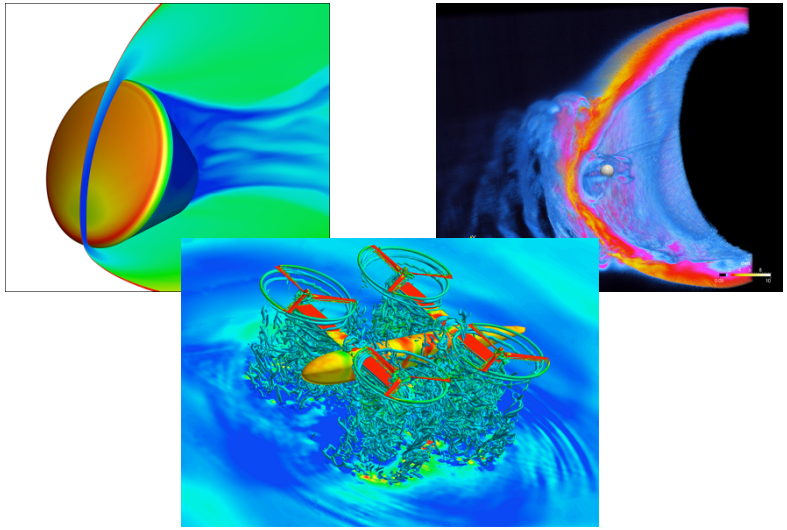
POC: Chris Shaw, robert.c.shaw@nasa.gov, (650) 604-4354, NASA Advanced Supercomputing Division, CSRA LLC

July 2016 Computer Usage on Pleiades Tops 20.7 Million SBUs

- July's computer usage on the Pleiades supercomputer set a new monthly record for the second month in a row.
- Over 20.75 million Standard Billing Units (SBUs*) were used by NASA's science and engineering organizations, exceeding by over 3 million the June 2016 record of 17.73 million SBUs.
- This increase was enabled by a second installation of 14 Broadwell racks (1008 nodes) that increased Pleiades' compute resources by 15%.
- Aeronautics Research Mission Directorate paid for 756 of these Broadwell nodes to increase the computing resources available to its scientists and engineers.
- Over 300 projects from all across NASA used time on Pleiades during July.
- 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) Visualization of temperature contours on the surface of the Orion spacecraft and Mach number contours on the symmetry plane. *C. Tang, NASA/Ames*. (2) Snapshot from a 3D global hybrid simulation of the Earth's magnetosphere. *M. Tatineni, San Diego Supercomputer Center & H. Karimabadi, U. of California, San Diego/ SciberQuest, Inc*. (3) Visualization of NASA's conceptual design of a large-scale quadrotor vehicle. *S. Yoon, NASA/Ames*.

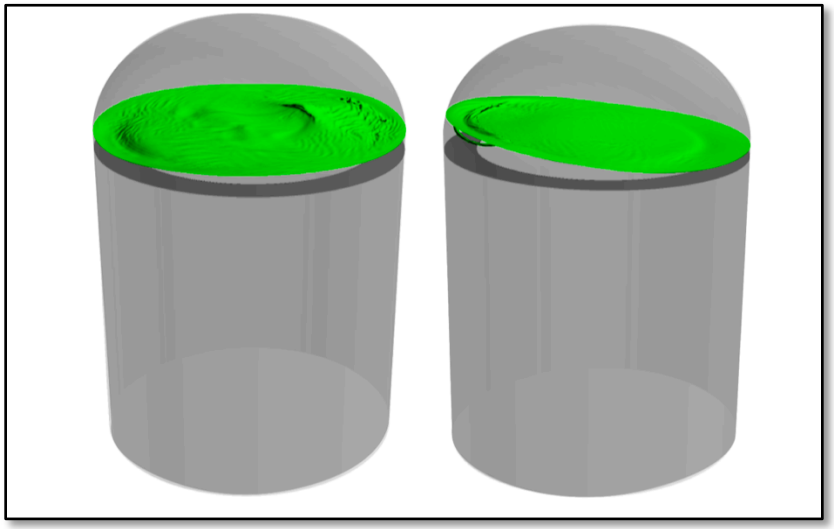
POC: Catherine Schulbach, catherine.h.schulbach@nasa.gov, (650) 604-3180, NASA Advanced Supercomputing Division

Pleiades Used to Predict Baffled Propellant Tank Slosh for Spacecraft *

- The motion of liquid propellant in a spacecraft fuel tank can interact with the vehicle's control system, causing a failure of structural components or deviation from its planned flight path. Computational fluid dynamics (CFD) researchers at NASA Marshall Space Flight Center (MSFC) are using Pleiades to accurately predict fuel slosh damping inside a baffled tank—baffles provide substantial damping when placed near the liquid surface.
- The research team validated MSFC's Loci-STREAM CFD solver against experimental test data for slosh damping inside a smooth-wall tank.
  - The team first used experimental data correlating with the industry standard for the smooth wall for a baseline validation.
  - Then they simulated damping due to baffle rings at different depths from the liquid surface—very good agreement with experimental data was observed.
- The simulations enabled by Pleiades demonstrate the reliability of the MSFC CFD approach in modeling the detailed fluid dynamics of tank sloshing, and the excellent accuracy in extracting slosh mechanical properties of slosh frequency, mass, and damping.
- Each simulation performed on Pleiades used 500 to 1,000 processors and ran for 1–3 days.

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

Mission Impact: HECC's Pleiades supercomputer is a critical resource for developing accurate methods to understand the physics behind spacecraft fuel slosh, accurately predicting slosh damping values, and validate CFD simulation results against experimental test data.



Liquid surface dynamics inside a propellant tank with an anti-slosh baffle. The submerged gas bubbles near the baffle surface and complex surface waves are visible.

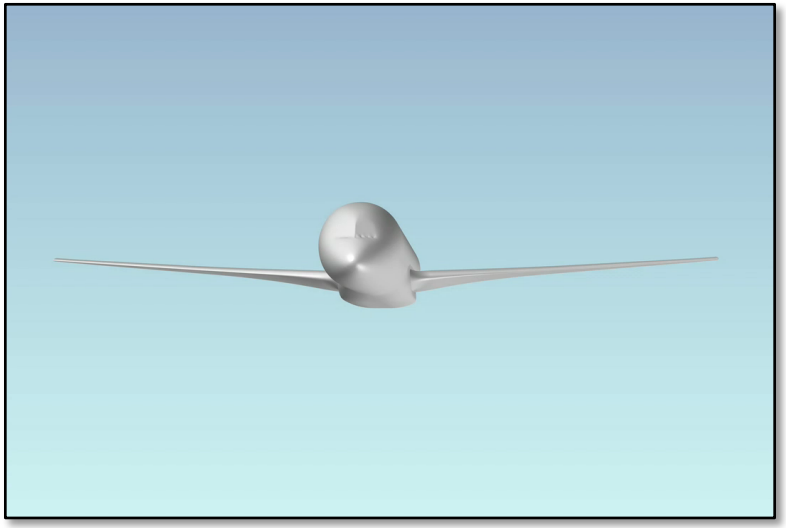
POCs: H. Q. Yang, hong.q.yang@nasa.gov, (256) 544-8979, Jeff West, jeffrey.s.west@nasa.gov, (256) 544-6309, NASA Marshall Space Flight Center

Endeavour Simulates the Use of Distributed Flaps to Optimize Flexible Wings During Flight *

- Aeronautics researchers at NASA Ames are running simulations on the Endeavour supercomputer to investigate the ability of a distributed flap system to improve aircraft performance and efficiency.
  - An aircraft's weight varies greatly as fuel burns, putting the wings at off-design conditions, especially in newer aircraft with composite, highly flexible wings.
  - The simulations help examine the potential of a full-span distributed flap system to adaptively reshape an aircraft wing to recover lost performance and keep the wing operating near peak efficiency throughout flight.
- This work combines aerodynamic shape optimization with structural modeling to optimize deflections of an array of 48 distributed flaps to reduce lift-induced drag. Results show:
  - A full-span flap system can manage the wing's lift distribution to achieve near-optimal performance throughout the cruise segment of the mission profile.
  - The system also shows great promise for reducing performance penalties from the strong wing shock when the aircraft is operating at off-design conditions.
- Next steps include evaluating other flap configurations to potentially reduce complexity without losing performance.

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

Mission Impact: HECC resources enabled these high-fidelity simulations and made it possible to quantify the benefits of distributed flaps in comparison with conventional aircraft, in support of NASA's Advanced Air Transportation Technology Project.



Animation of a full-span distributed flap system installed on a generic transport aircraft with a highly flexible wing. Simulations help analyze the system's potential to adaptively reshape the wing in order to recover lost performance and keep the wing operating near peak efficiency. *David L. Rodriguez, NASA/Ames* (*Zoom in to view video details.*)

POCs: David L. Rodriguez, david.l.rodriguez@nasa.gov, (650) 604-0884, NASA Advanced Supercomputing (NAS) Division, Science and Technology Corp; Michael Aftosmis, michael.aftosmis@nasa.gov, (650) 604-4499, NAS Division

HECC Facility Hosts Several Visitors and Tours in July 2016

- HECC hosted 15 tour groups in July; guests learned about the agency-wide missions being supported by HECC assets, and some groups also viewed the D-Wave 2X quantum computer system. Visitors this month included:
  - Kim Toufectis, NASA agency master planner.
  - Norman Mineta, former U.S. Secretary of Transportation and former Secretary of Commerce.
  - Sue Bussells, U.S. Department of Agriculture deputy chief information officer and chief data officer.
  - Twenty members of the Scientific and Technical Information (STI) program.
  - Thirty interns from the Naval Postgraduate School.
  - Twenty interns from the Army High-Performance Computing Research Center Summer Institute at Stanford University.
  - Sixty Ames summer interns.
  - Ten teachers from the Ames 21st Century Teacher Summer Academy.

Norman Mineta (front row, center), former U.S. Secretary of Transportation and former Secretary of Commerce, received an overview of science and engineering work being done at the NAS facility from Piyush Mehrotra, Chief, NASA Advanced Supercomputing Division (not pictured). Interns from the Naval Postgraduate School joined Mineta on the tour.

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

Papers

- "**Progress Towards Physics-Based Space Weather Forecasting with Exascale Computing**," M. Innocenti, A. Johnson, S. Markidis, J. Deca, V. Olshevsky, G. Lapenta, Advances in Engineering Software, July 6, 2016. * *http://www.sciencedirect.com/science/article/pii/S0965997816301363*
- "**Neptune's Orbital Migration was Grainy, Not Smooth**," D. Nesvorny, D. Vokrouhilcky, The Astrophysical Journal, vol. 825, no. 2, July 6, 2016. * *http://iopscience.iop.org/article/10.3847/0004-637X/825/2/94/meta*
- "**An Entropy-Residual Shock Detector for Solving Conservation Laws Using High-Order Discontinuous Galerkin Methods**," Y. Lv, Y.-C. See, M. Ihme, Journal of Computational Physics, vol. 322, available online July 7, 2016. * *http://www.sciencedirect.com/science/article/pii/S0021999116302777*
- "**A Global Model for Circumgalactic and Cluster-Core Precipitation**," G. Voit, G. Meece, Y. Li, B. O'Shea, M. Donahue, arXiv:1607.022212 [astro-ph.GA], July 8, 2016. * *http://arxiv.org/abs/1607.02212*
- "**A Low Upper Limit on the Subsurface Rise Speed of Solar Active Regions**," A. Birch, H. Schunker, D. Braun, R. Cameron, L. Gizon, B. Loptien, M. Rempel, Science Advances, vol. 2, no. 7, July 13, 2016. * *http://advances.sciencemag.org/content/2/7/e1600557.abstract*

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

Papers (cont.)

- "**Influence of Measurement Uncertainties on Fractional Solubility of Iron in Mineral Aerosols Over the Oceans**," N. Meskhidze, M. Johnson, D. Hurley, K. Dawson, Aeolian Research, vol. 22, available online July 25, 2016. *
  http://www.sciencedirect.com/science/article/pii/S1875963716300374
- "**Numerical Evaluation of an Ejector-Enhanced Resonant Pulse Combustor with a Poppet Inlet Valve and a Converging Exhaust Nozzle**," S. Yungster, D. Paxson, H. Perkins, presented at the 52nd AIAA/SAE/Joint Propulsion Conference, Propulsion and Energy Forum, July 25-27, 2016. *
  http://arc.aiaa.org/doi/abs/10.2514/6.2016-4559
- "**CFD Analysis of Mixing Characteristics of Several Fuel Injectors at Hypervelocity Flow Conditions**," T. Drozda, J. P. Drummond, R. Baurle, presented at the 52nd AIAA/SAE/ Joint Propulsion Conference, Propulsion and Energy Forum, July 25-27, 2016. *
  http://arc.aiaa.org/doi/abs/10.2514/6.2016-4764
- "**Enhancement of the Open National Combustor Code (Open NCC) and Initial Simulation of Energy Efficient Engine**," K. Miki, J. Moder, M.-S. Liou, presented at the 52nd AIAA/SAE/Joint Propulsion Conference, Propulsion and Energy Forum, July 25-27, 2016. *
  http://arc.aiaa.org/doi/abs/10.2514/6.2016-4651

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

Papers (cont.)

- "**Numerical Investigation of Shrouded Ejector-Enhanced Pulse Combustor Performance at High Pressure**," S. Yungster, D. Paxon, H. Perkins, presented at the 52nd AIAA/SAE/Joint Propulsion Conference, Propulsion and Energy Forum, July 25-27, 2016. * *http://arc.aiaa.org/doi/abs/10.2514/1.B36082*
- "**Changes in Growing Season Duration and Productivity of Northern Vegetation Inferred from Long-Term Remote Sensing Data**," T. Park, S. Ganguly, R. Nemani, et al., Environmental Research Letters, vol. 11, no. 8, July 27, 2016. *http://iopscience.iop.org/article/10.1088/1748-9326/11/8/084001/meta*
- "**The Orbital Distribution of Trans-Neptunian Objects Beyond 50 au**," D. Nesvorny, D. Vokrouhlicky, F. Roig, arXiv:1607.08279 [astro-ph.EP], July 27, 2016. * *http://arxiv.org/abs/1607.08279*

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

Presentations

- "**A DSMC Surface Chemistry Model for Carbon-Based Ablators**," A. Borner, K. Gopalan, K. Stephani, N. Mansour, presented at the 30th International Symposium on Rarefield Gas Dynamics, Victoria, British Columbia, July 10–15, 2016.*
- "**Early Solar Cycle Prediction with the Data Assimilation Approach: Uncertainties and Future Challenges**," I. Kitiashvili, Solar Heliophysics and Interplanetary Environment Meeting, Santa Fe, AZ, July 11–15, 2016.*
- "**3D Realistic MHD Modeling of Solar Activity in Quiet-Sun Regions**," I. Kitiashvili, A. Kosovichev, N. Mansour, A. Wray, Solar Heliophysics and Interplanetary Environment Meeting, Santa Fe, NM, July 11–15, 2016.*

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

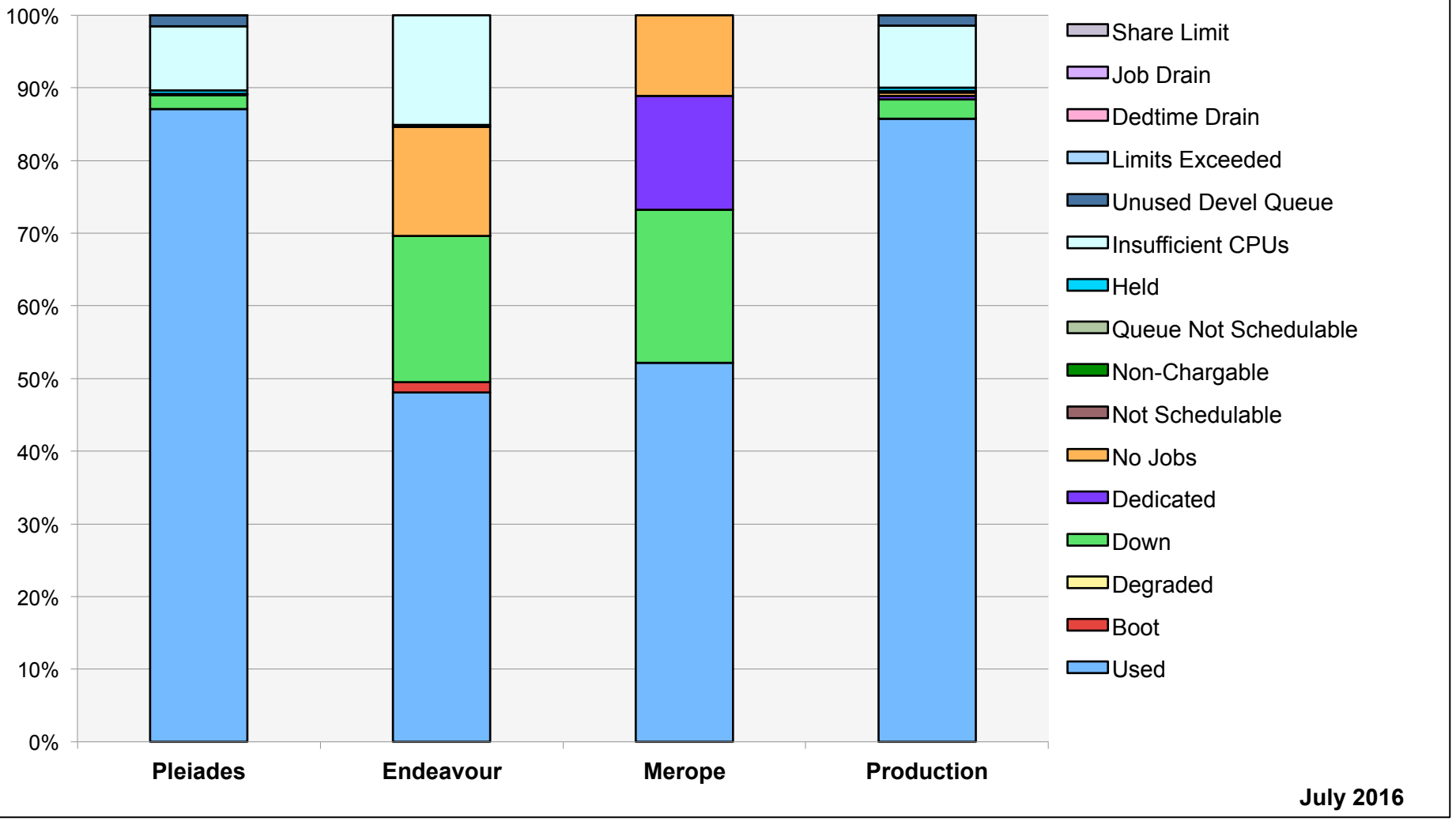
News and Events

- **Discovering the Origin of Stars Through 3D Simulation**, *NAS feature*, June 30, 2016—Astrophysicists at the University of California, Berkeley and Lawrence Livermore National Laboratory (LLNL) created a first-of-a-kind simulations run on the Pleiades supercomputer to piece together the origin of stars, stellar clusters, and the high-mass stars that form within them.
  http://www.nas.nasa.gov/publications/articles/feature_origin_of_stars_Klein.html
  - **3-D Simulations and NASA Supercomputer Help Further Discovery of the Origin of Stars**, *NASA Ames feature*, July 6, 2016.
    https://www.nasa.gov/feature/ames/3-d-simulations-and-nasa-supercomputer-help-further-discovery-of-the-origin-of-stars
  - **NASA's Newly Upgraded Pleiades Supercomputer Delves into the Mysteries of Stars Formation**, *TechCrunch*, July 6, 2016.
    https://techcrunch.com/2016/07/06/nasas-newly-upgraded-pleiades-supercomputer-delves-into-the-mysteries-of-star-formation/
  - **3-D Simulations and NASA Supercomputer Advance Research of the Origin of Stars**, *PhysOrg*, July 7, 2016.
    http://phys.org/news/2016-07-d-simulations-nasa-supercomputer-advance.html
  - **A Ringside Seat at the Birth of Stars**, *Cosmos Magazine*, July 7, 2016.
    https://cosmosmagazine.com/technology/supercomputer-simulation-takes-us-back-hundreds-of-thousands-of-years
  - **Star-Maker**, *Slate*, July 17, 2016.
    http://www.slate.com/articles/video/video/2016/07/watch_stellar_nurseries_form_in_a_hypnotic_new_3_d_simulation_video.html (Flash Player)

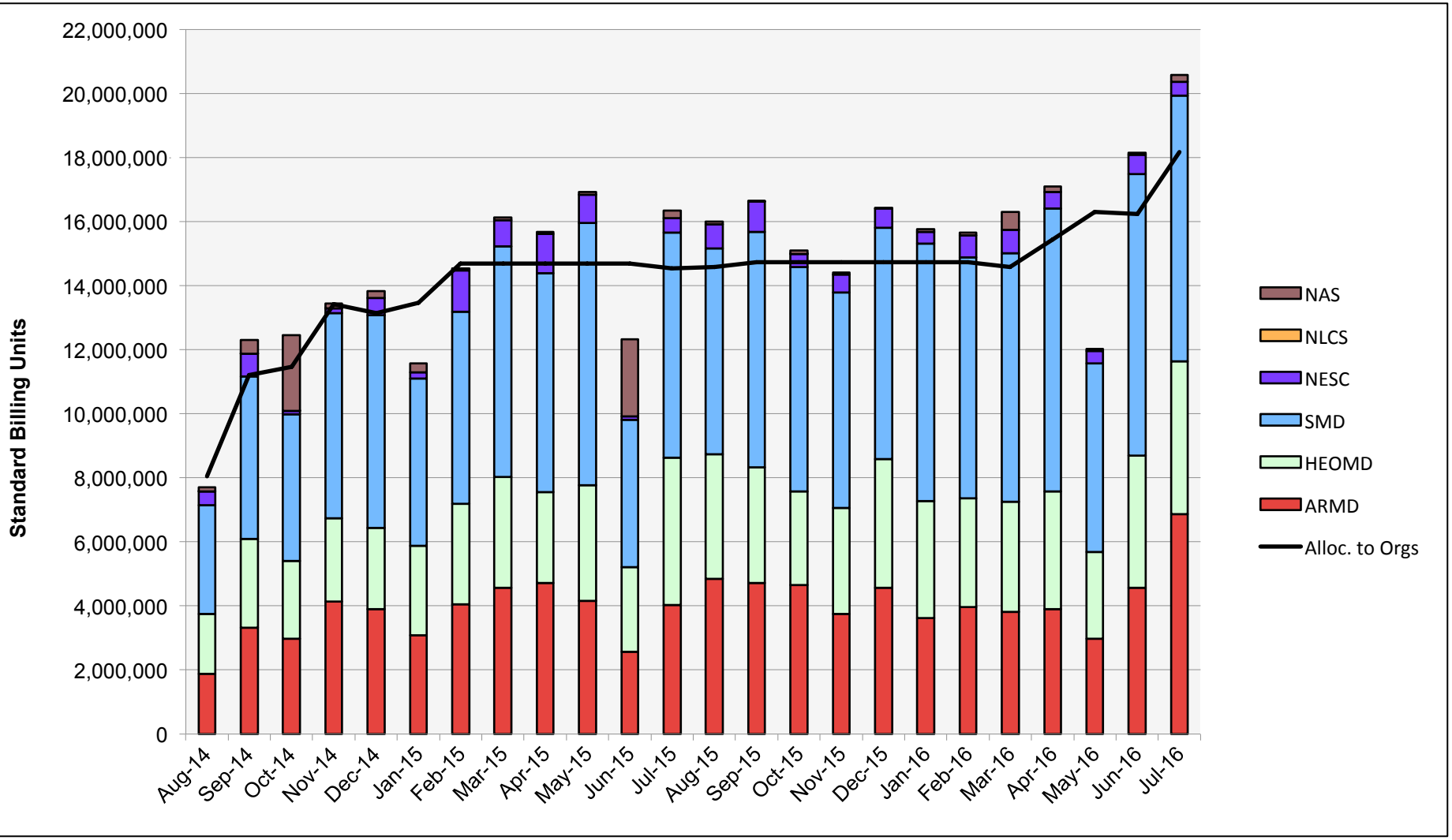
News and Events (cont.)

- **Slow Appearance of Sunspots Challenges Theory**, *Max Planck Institute for Solar System Research news announcement,* July 13, 2016—Using the Pleiades supercomputer and images from NASA's Solar Dynamics Observatory, MPS scientists published a paper in the Journal *Science Advances* showing that magnetic flux concentrations move upward through the solar interior at speeds much slower than predicted by the prevailing current model.
  http://www.mps.mpg.de/slow-appearance-of-sunspots-challenges-theory
- **NASA Boosts Pleiades Supercomputer with Broadwell CPUs and LTO Tape**, *insideHPC*, July 15, 2016—The NASA Advanced Supercomputing Division augmented the flagship Pleiades supercomputer with 14 racks of Intel Xeon "Broadwell" processors, increasing the system's theoretical peak performance to 7.25 petaflops.
  http://insidehpc.com/2016/07/pleiades/

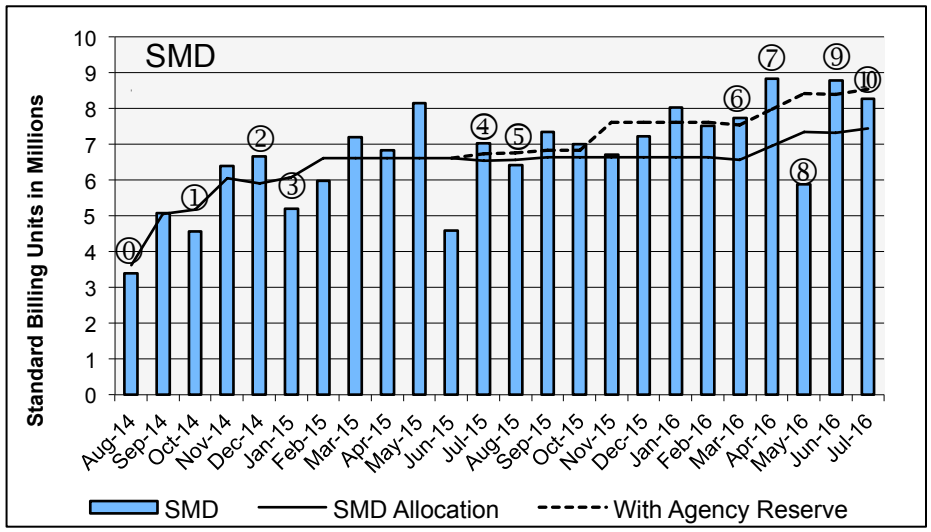
HECC Utilization

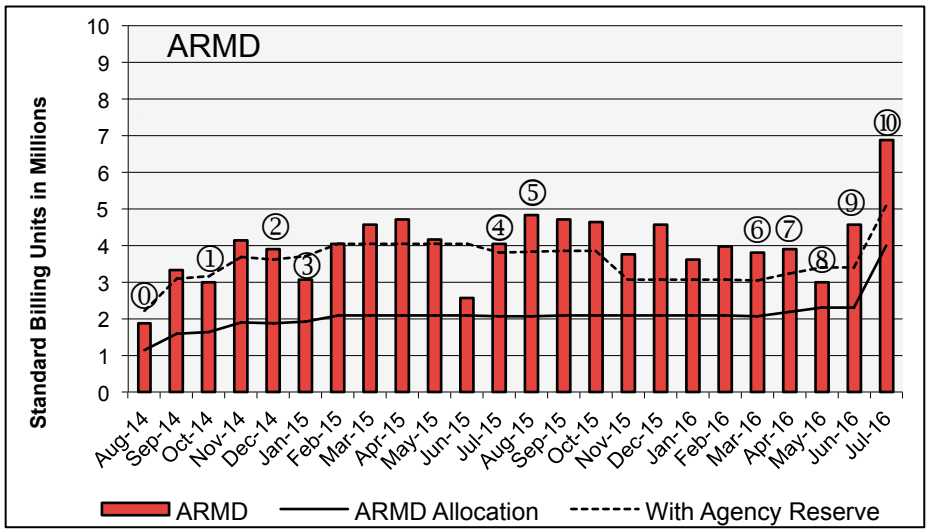


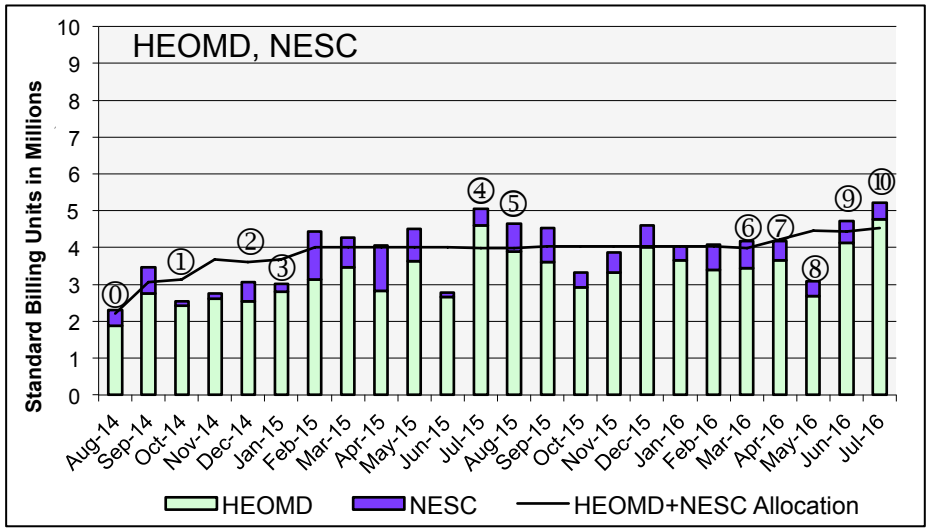
HECC Utilization Normalized to 30-Day Month



HECC Utilization Normalized to 30-Day Month

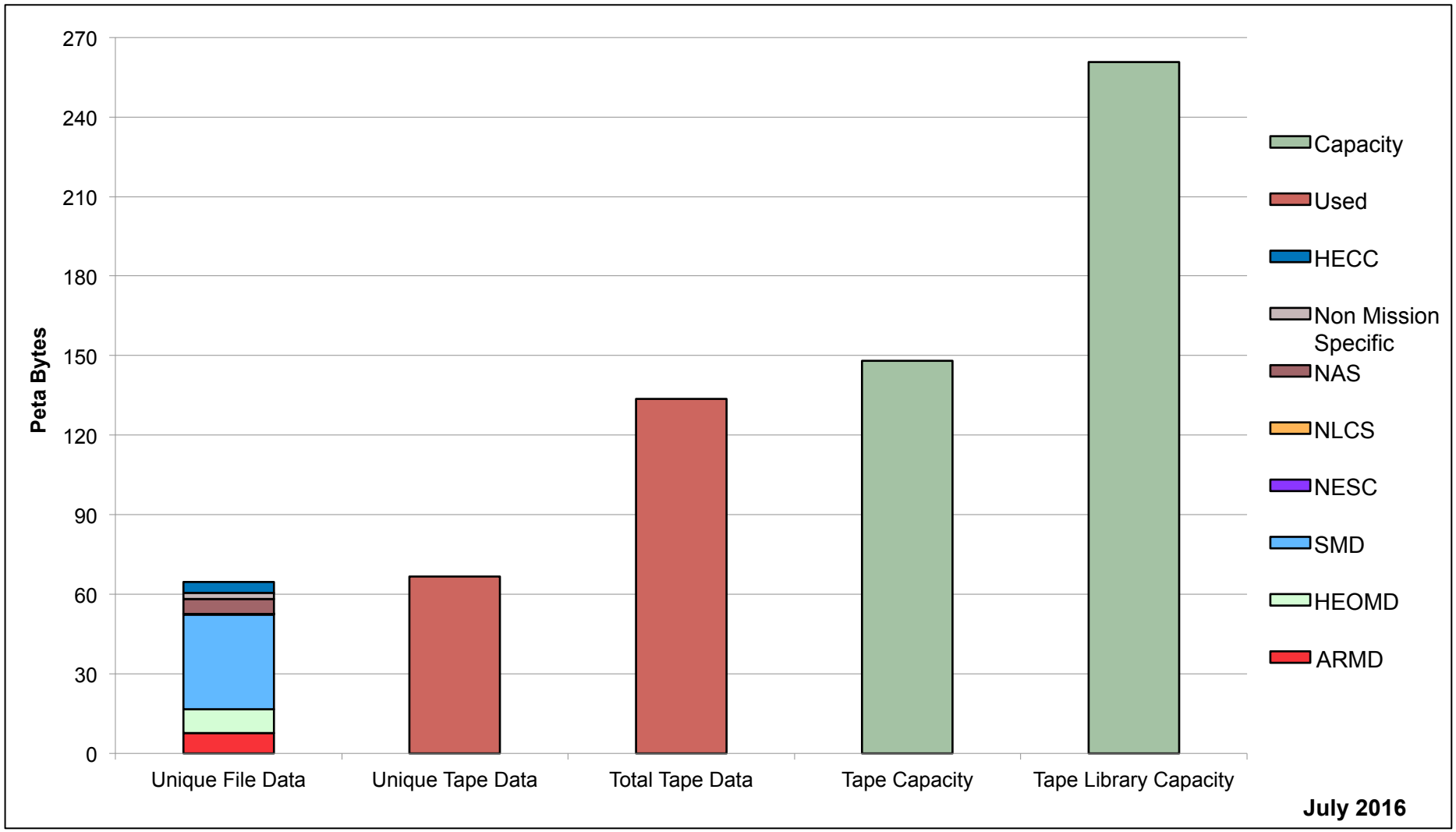




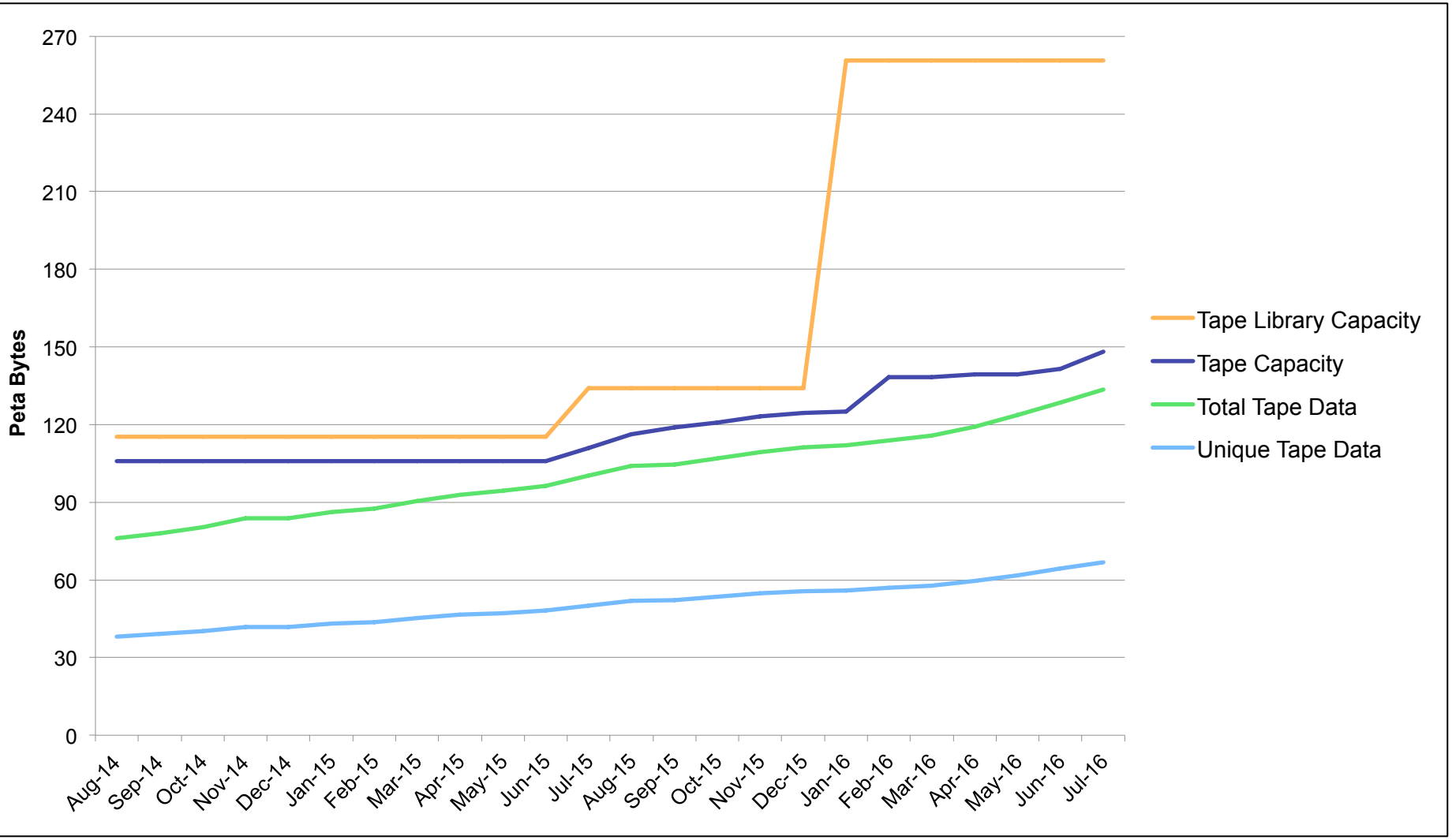


⓪ 6 Westmere ½ racks added to Merope, 6 Harpertown ½ racks retired from Merope
① 16 Westmere racks retired from, 3 Ivy Bridge and 15 Haswell racks added to Pleiades; 10 Nehalem and 2 Westmere racks added to Merope
② 16 Westmere racks retired from Pleiades
③ 14 Haswell racks added to Pleiades
④ 7 Nehalem 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)

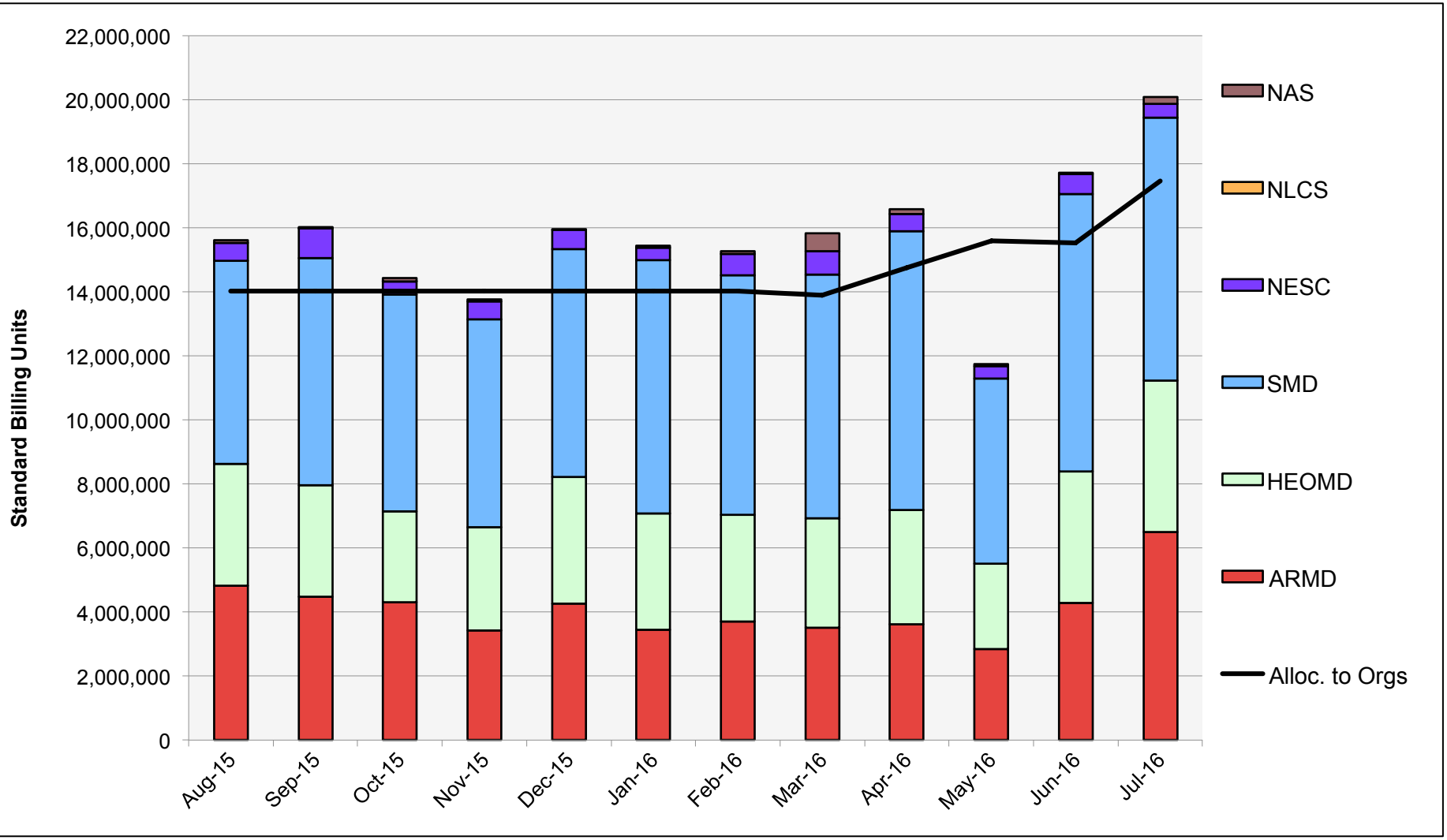
Tape Archive Status



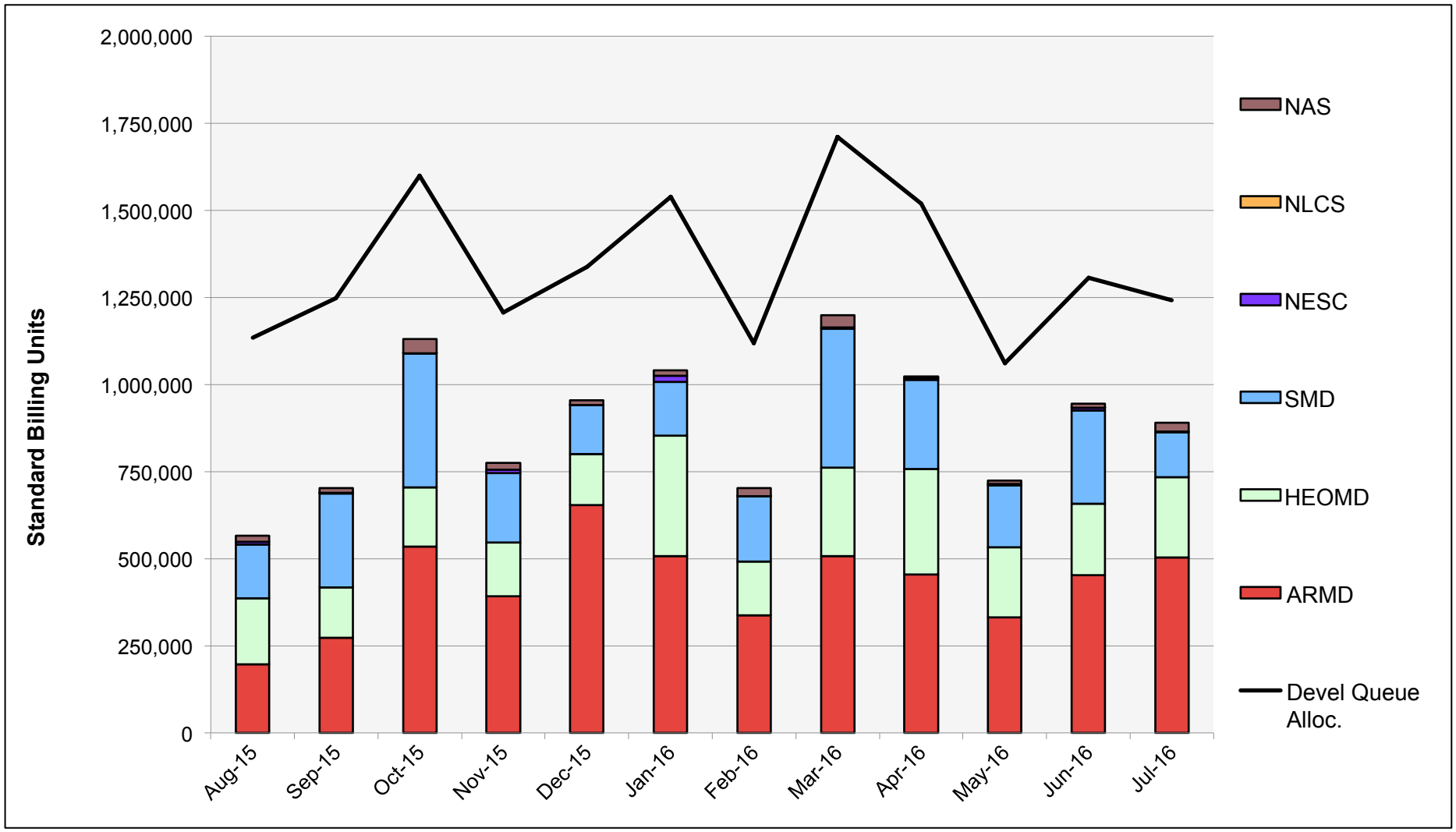
Tape Archive Status



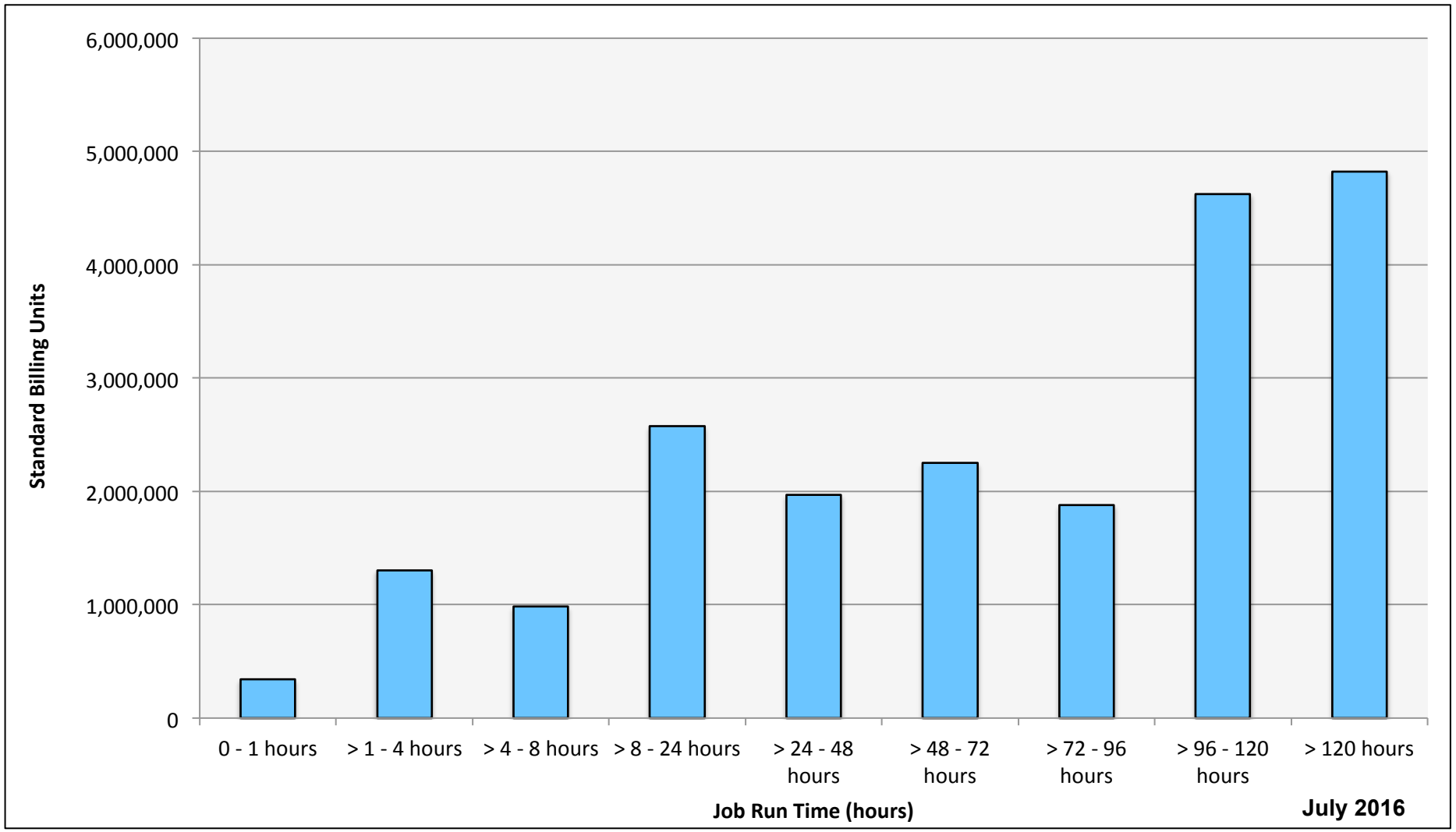
Pleiades:
SBUs Reported, Normalized to 30-Day Month



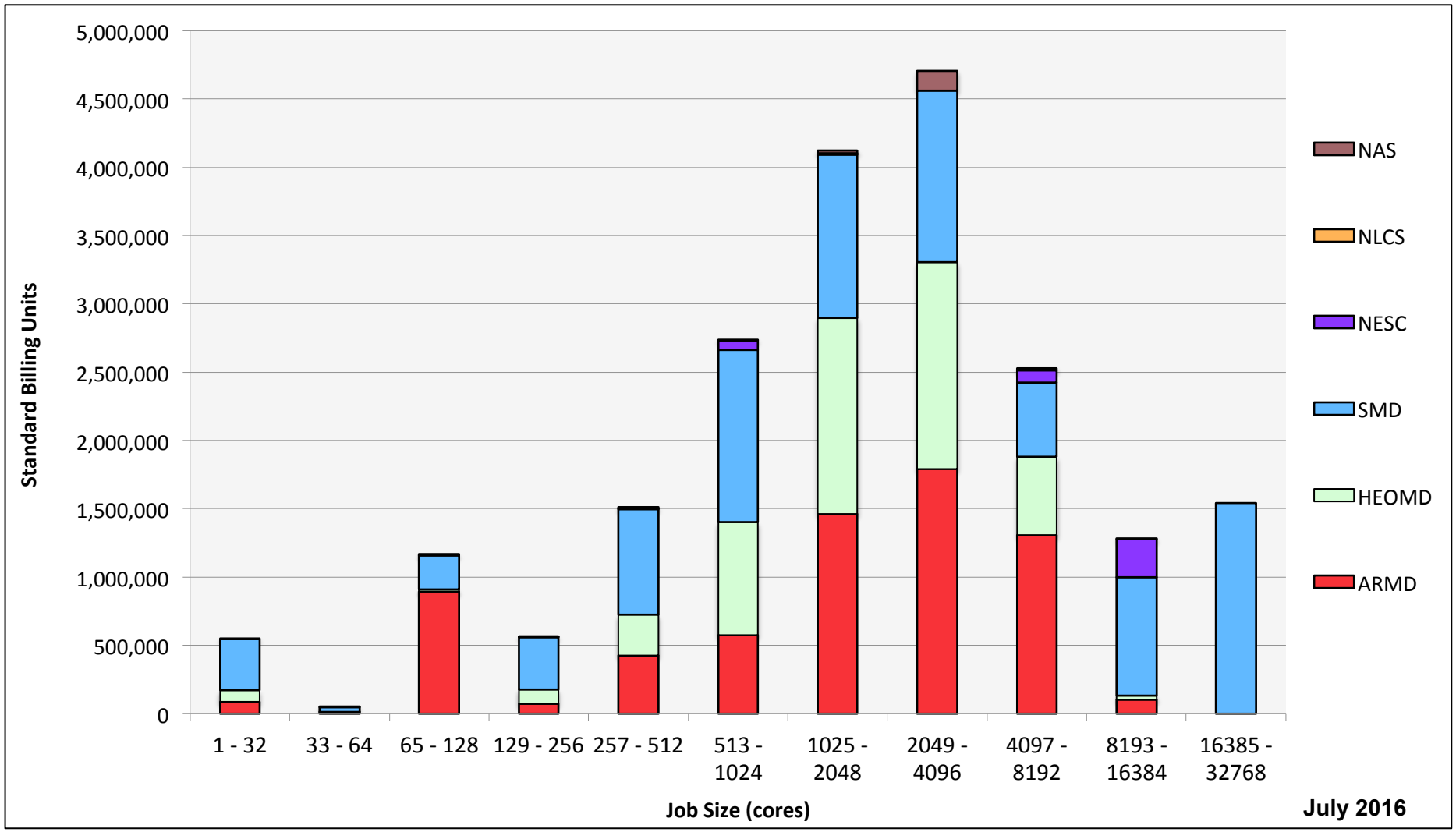
Pleiades:
Devel Queue Utilization



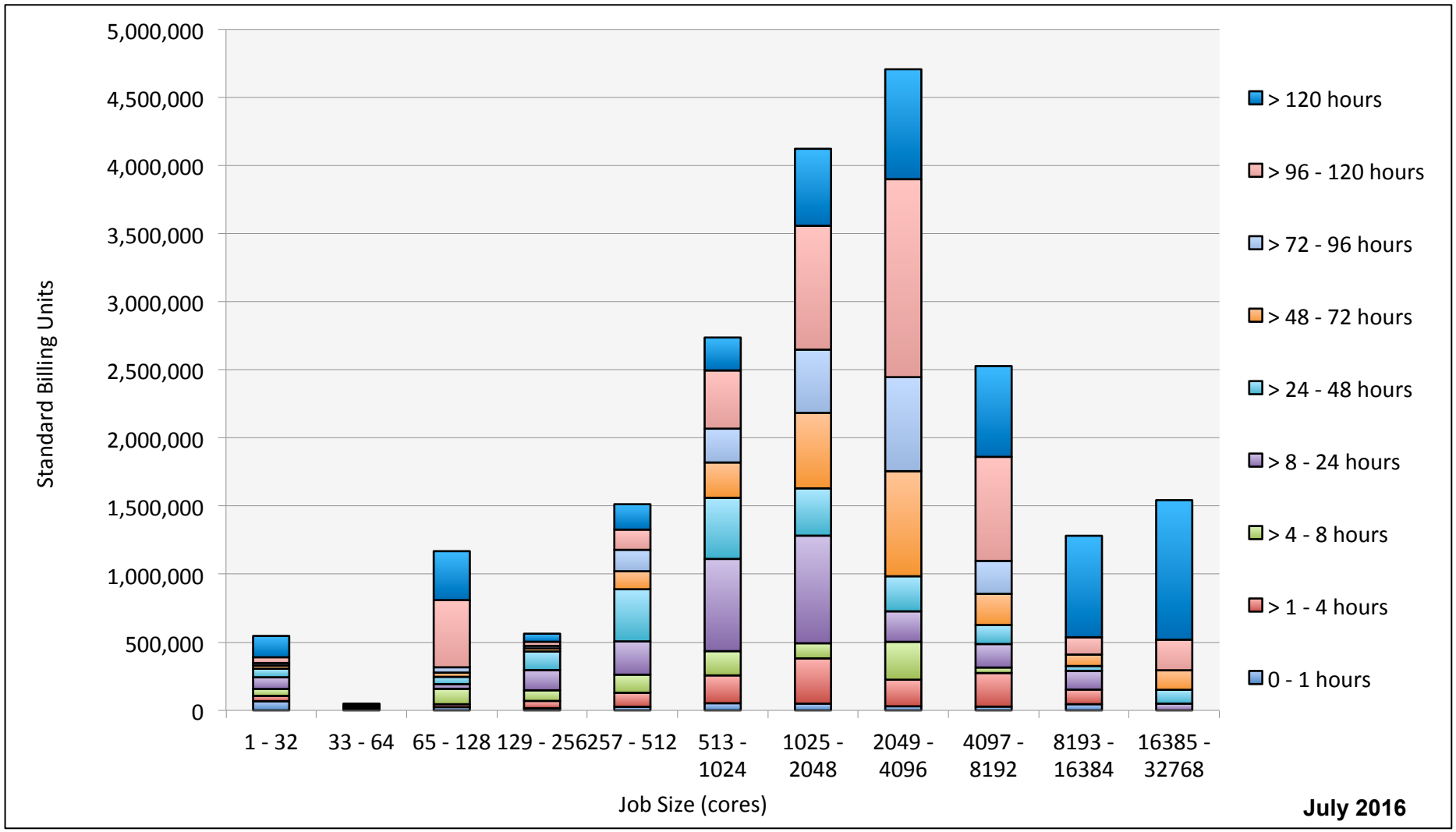
Pleiades:
Monthly Utilization by Job Length



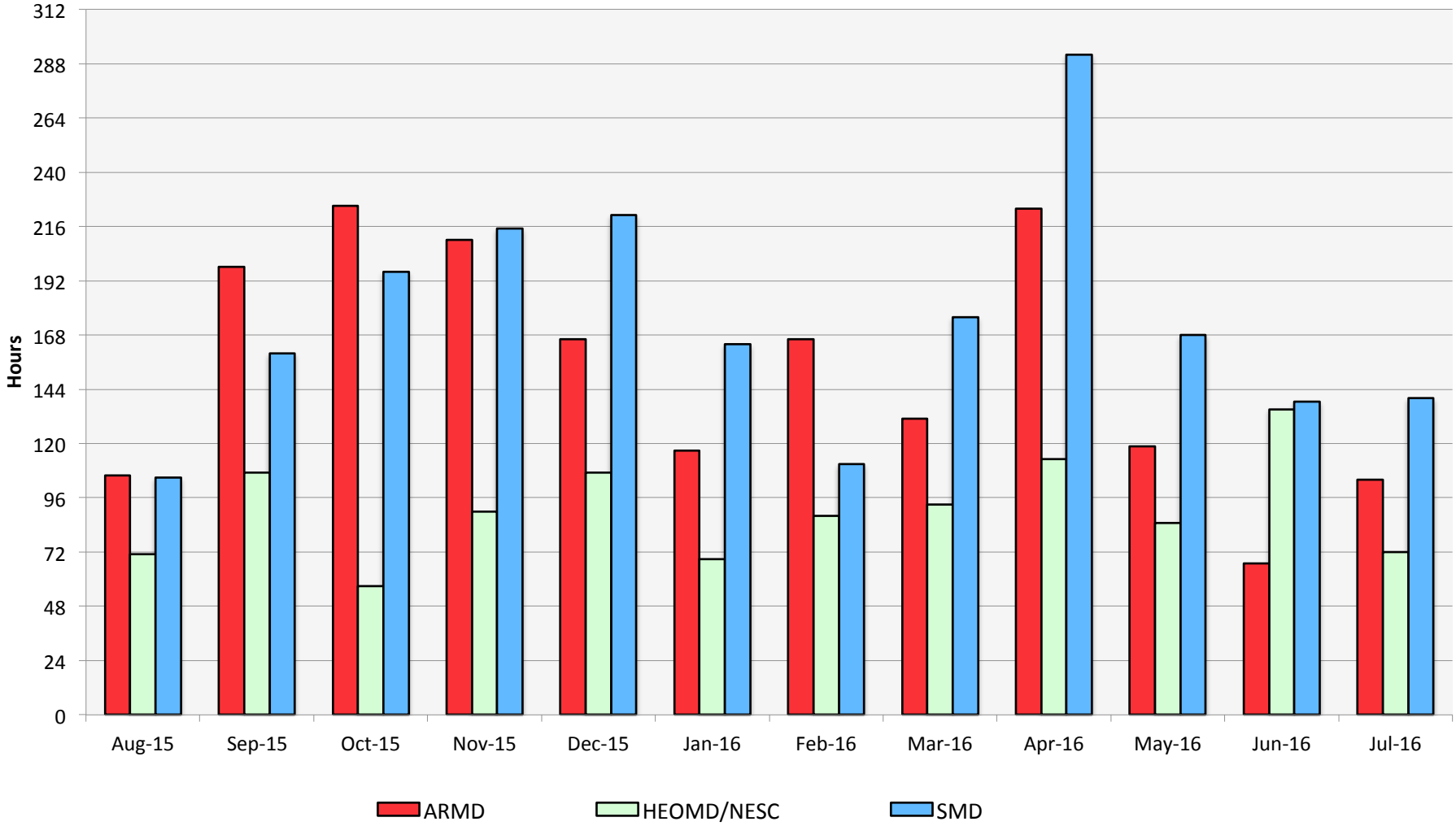
Pleiades:
Monthly Utilization by Size and Mission



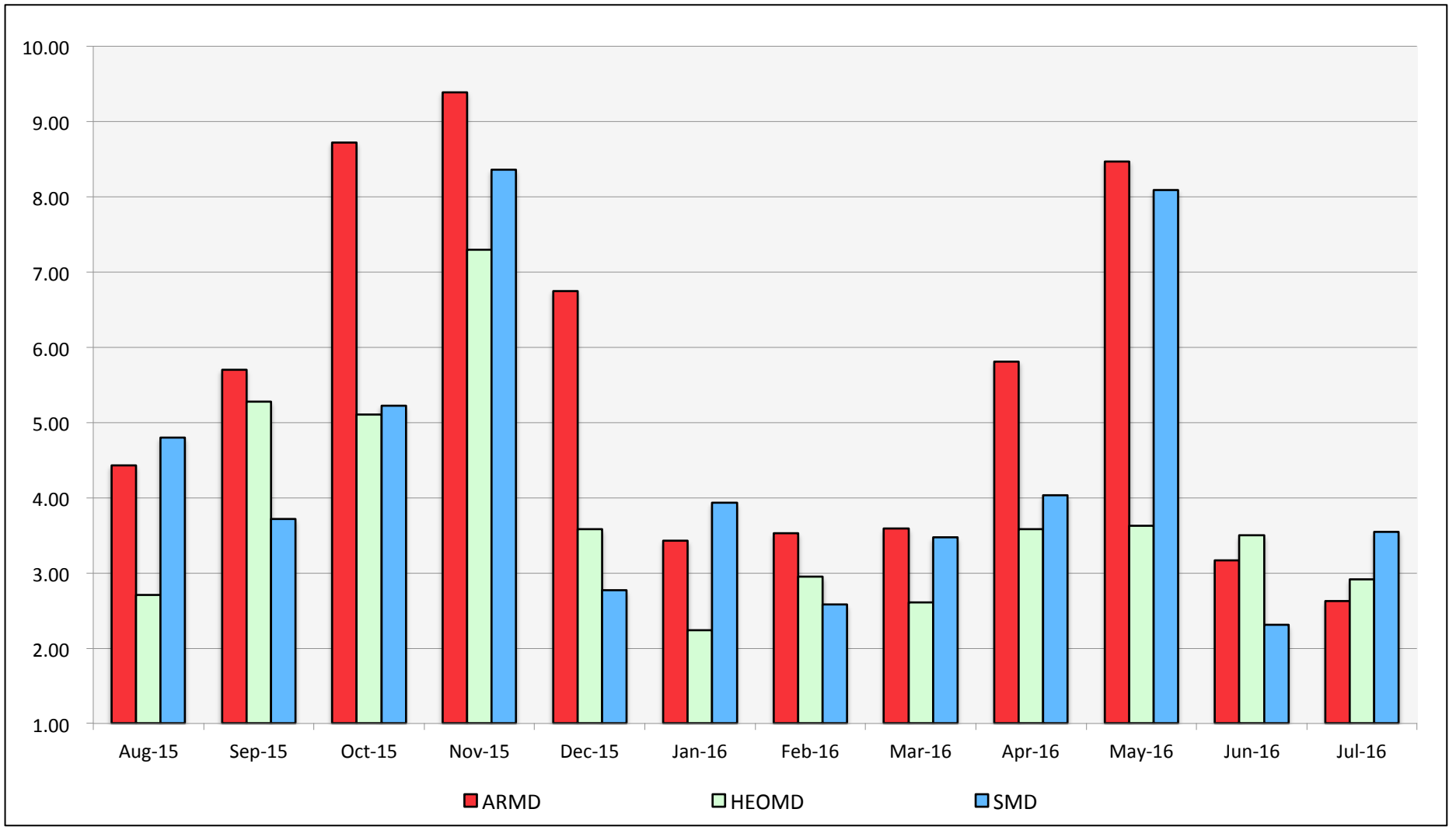
Pleiades:
Monthly Utilization by Size and Length



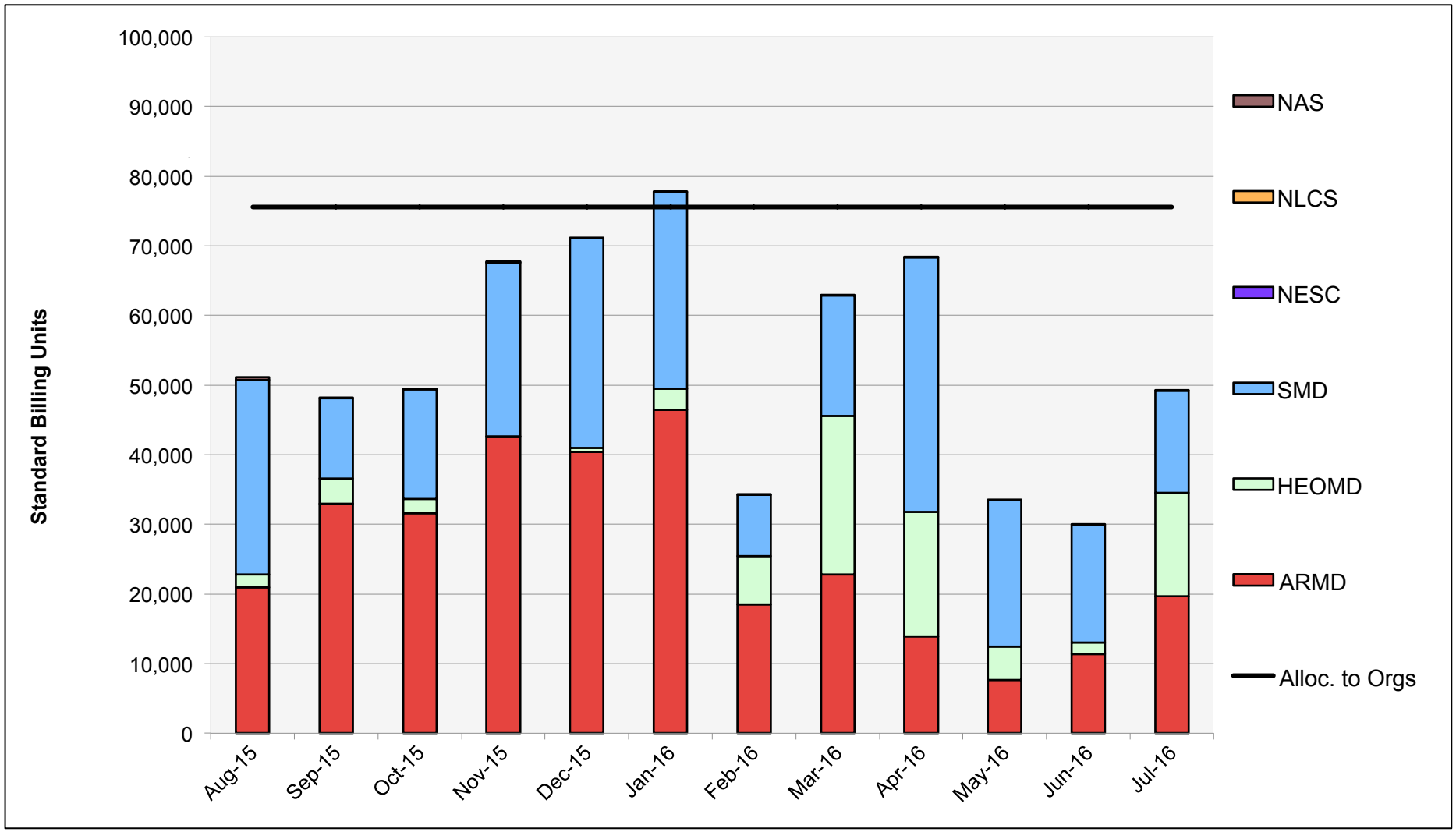
Pleiades:
Average Time to Clear All Jobs



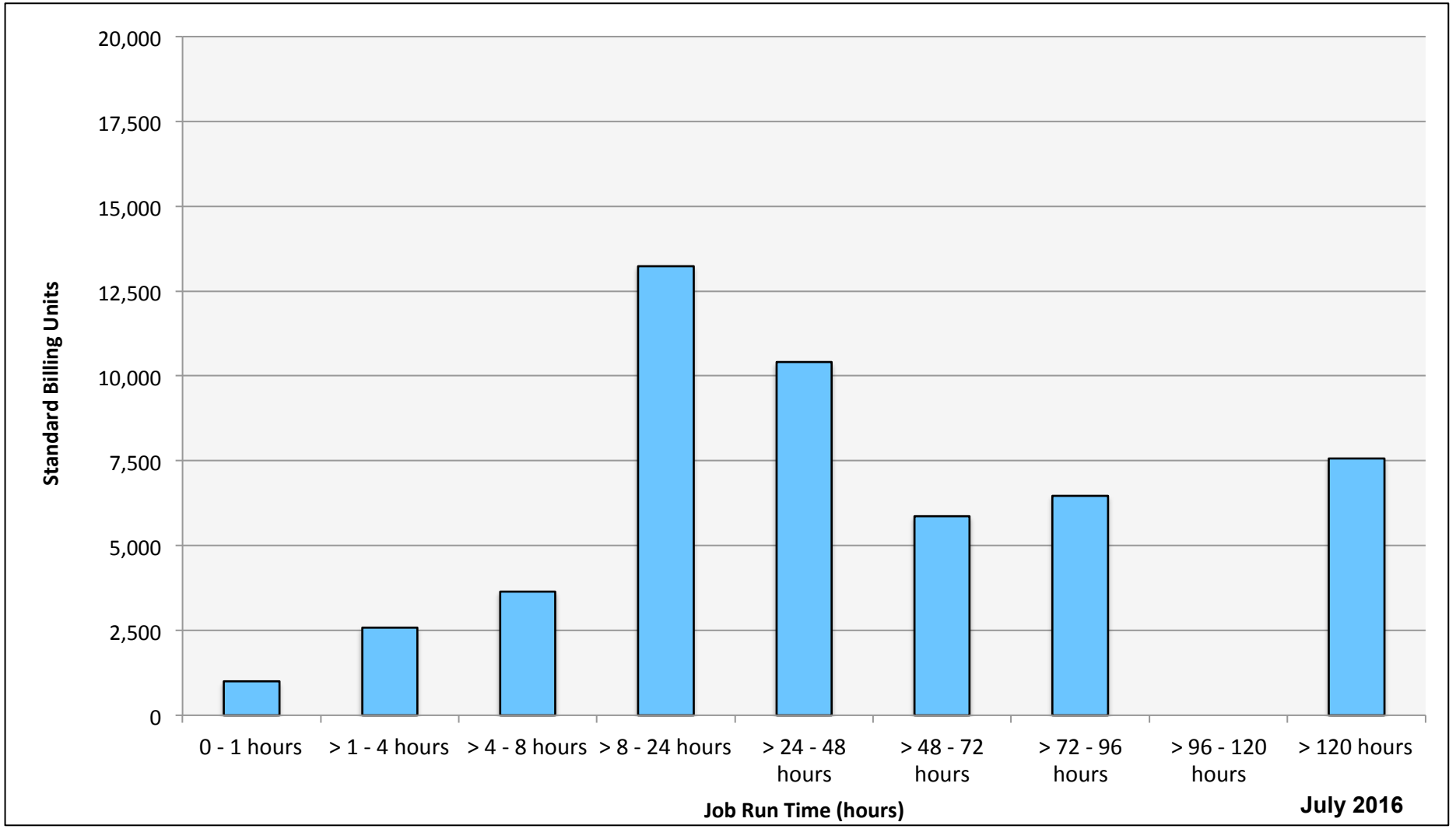
Pleiades:
Average Expansion Factor



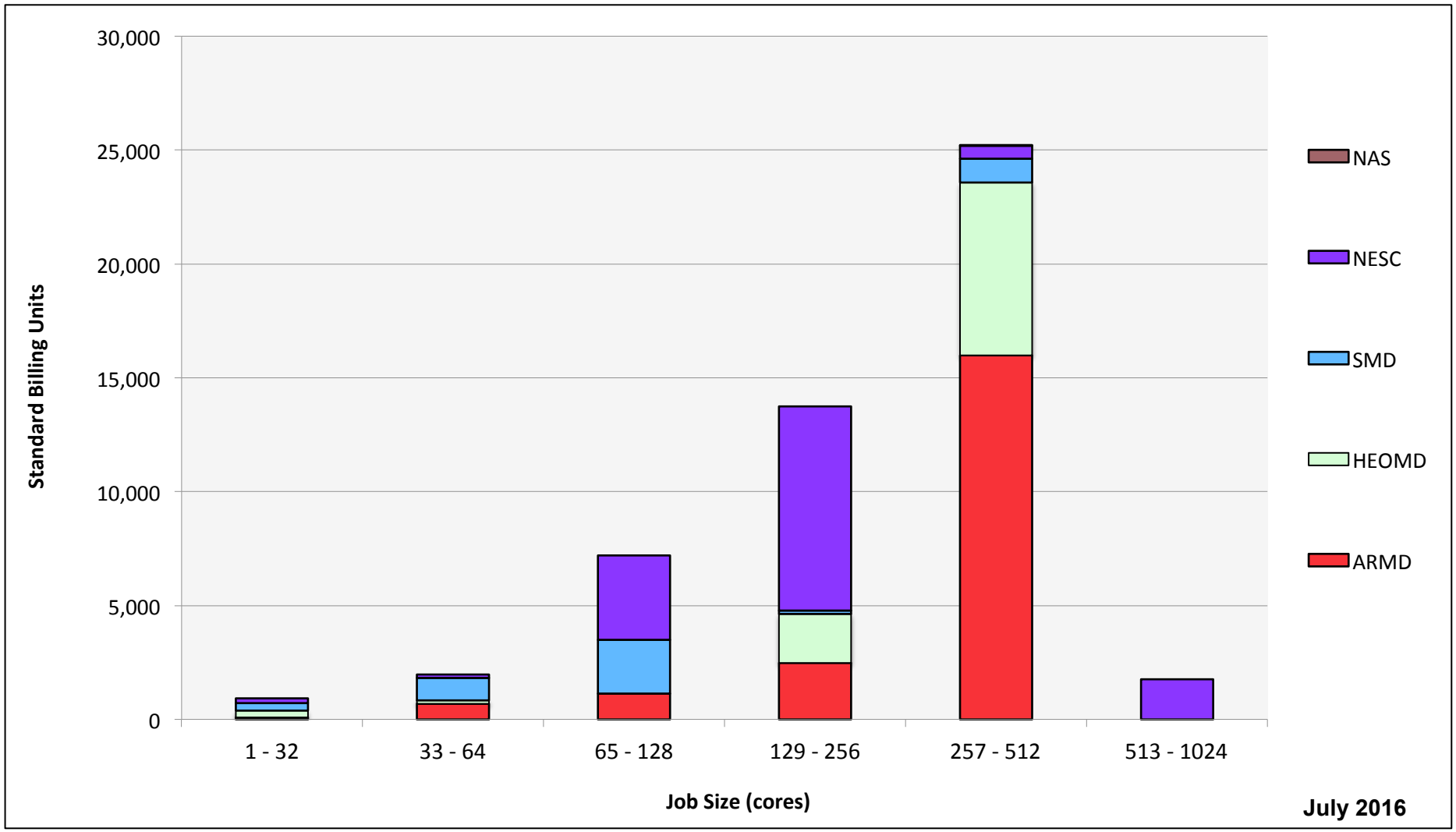
Endeavour:
SBUs Reported, Normalized to 30-Day Month



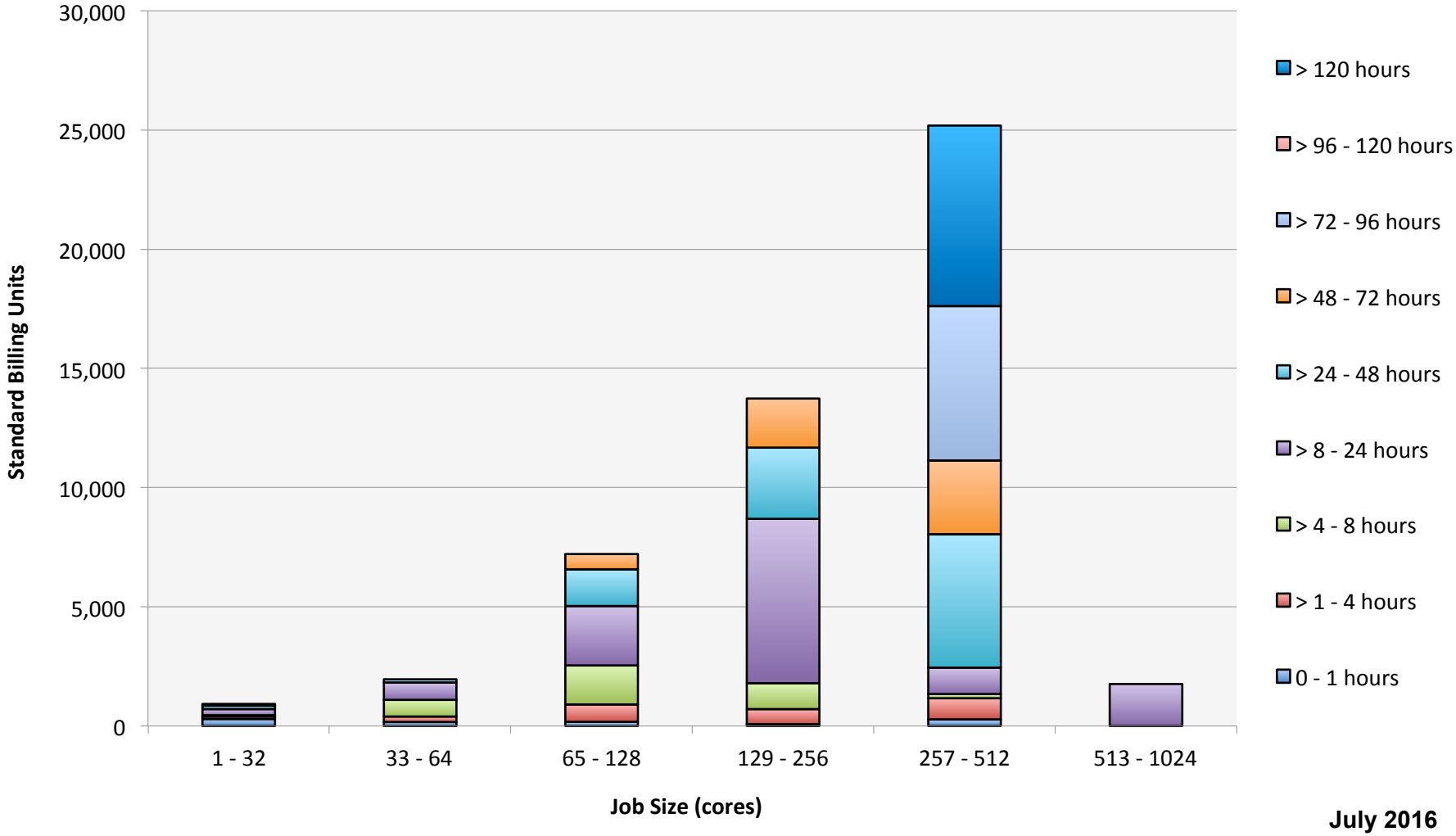
Endeavour:
Monthly Utilization by Job Length



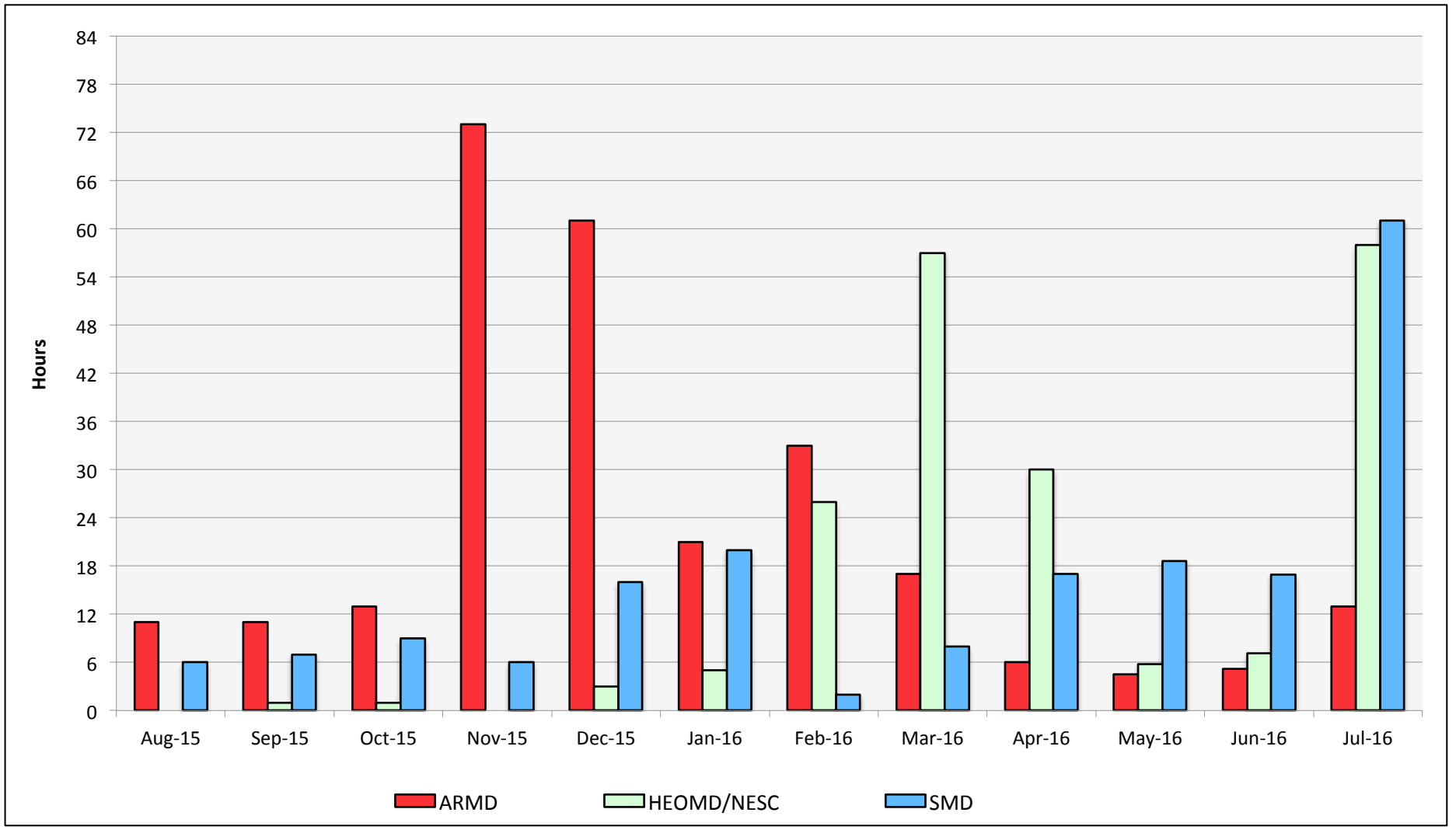
Endeavour:
Monthly Utilization by Size and Mission



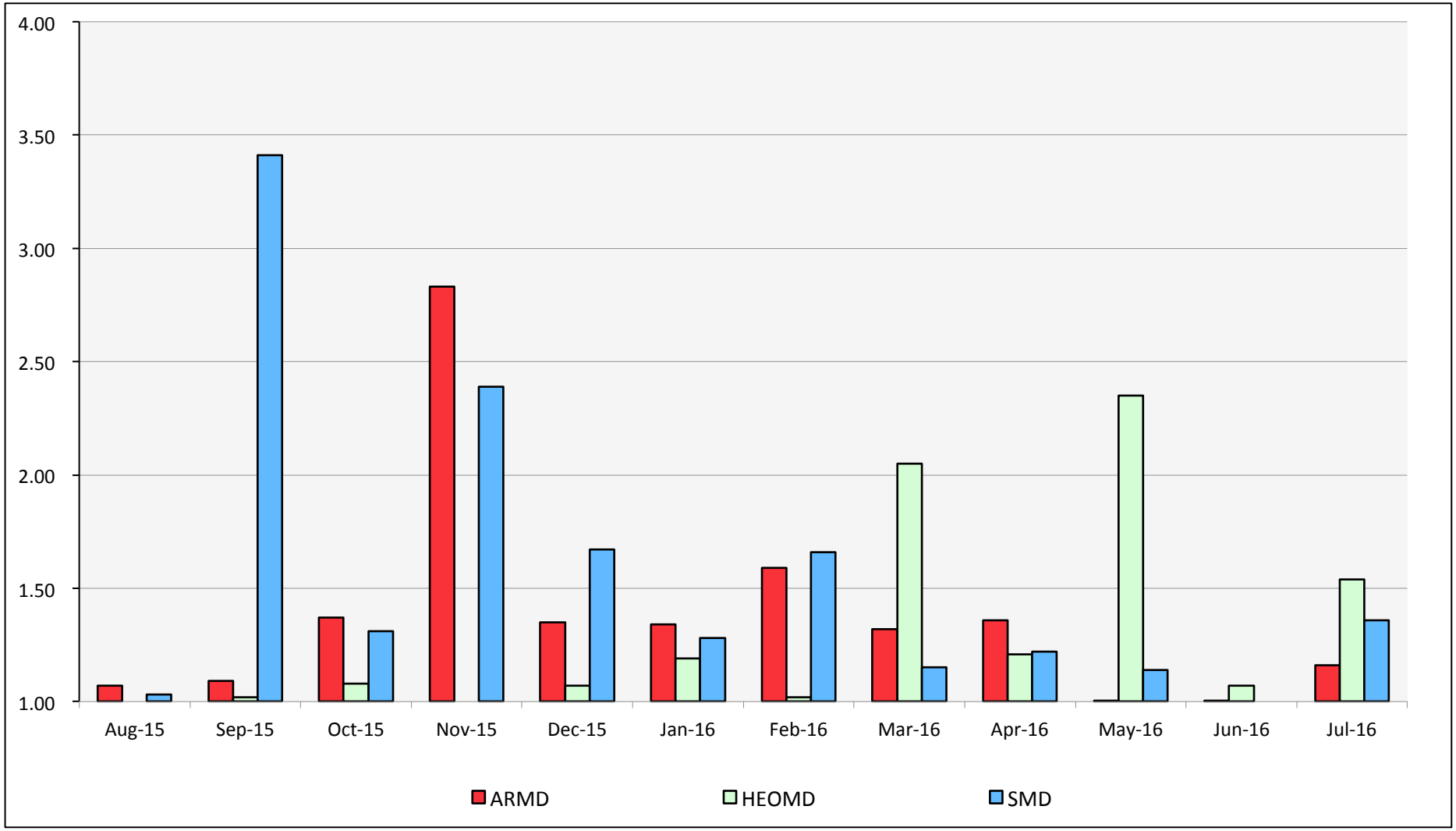
Endeavour:
Monthly Utilization by Size and Length



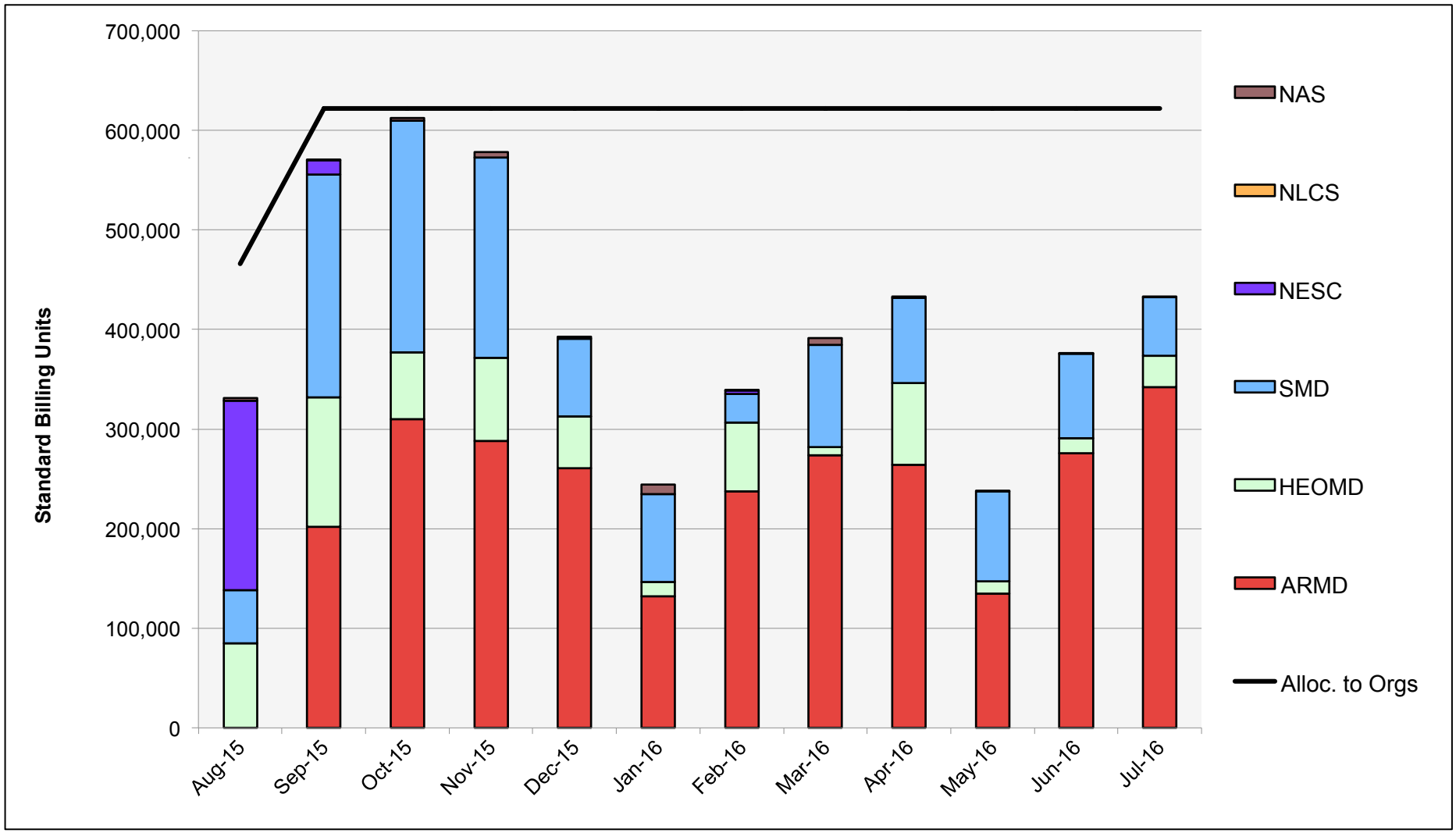
Endeavour:
Average Time to Clear All Jobs



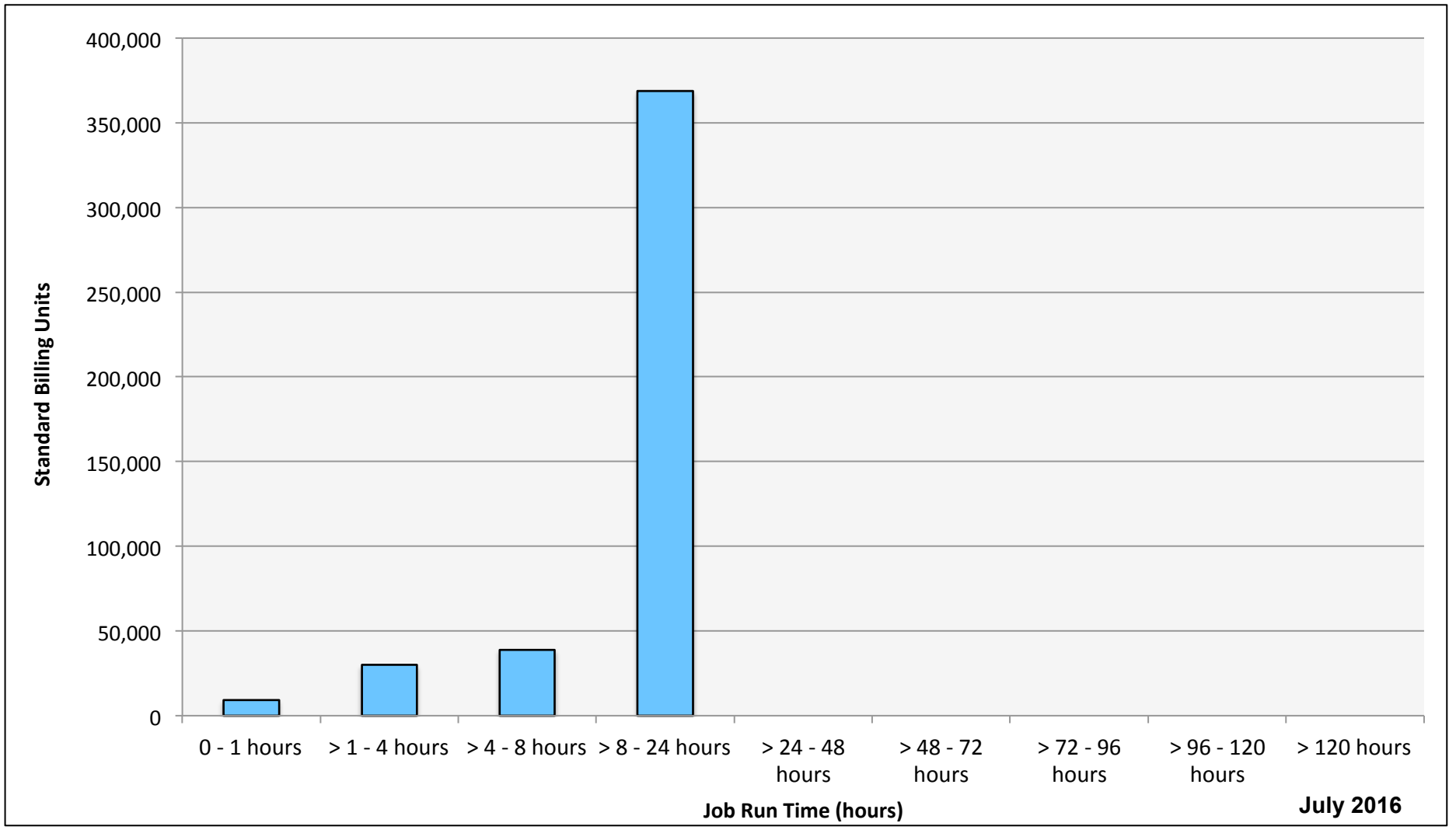
Endeavour:
Average Expansion Factor



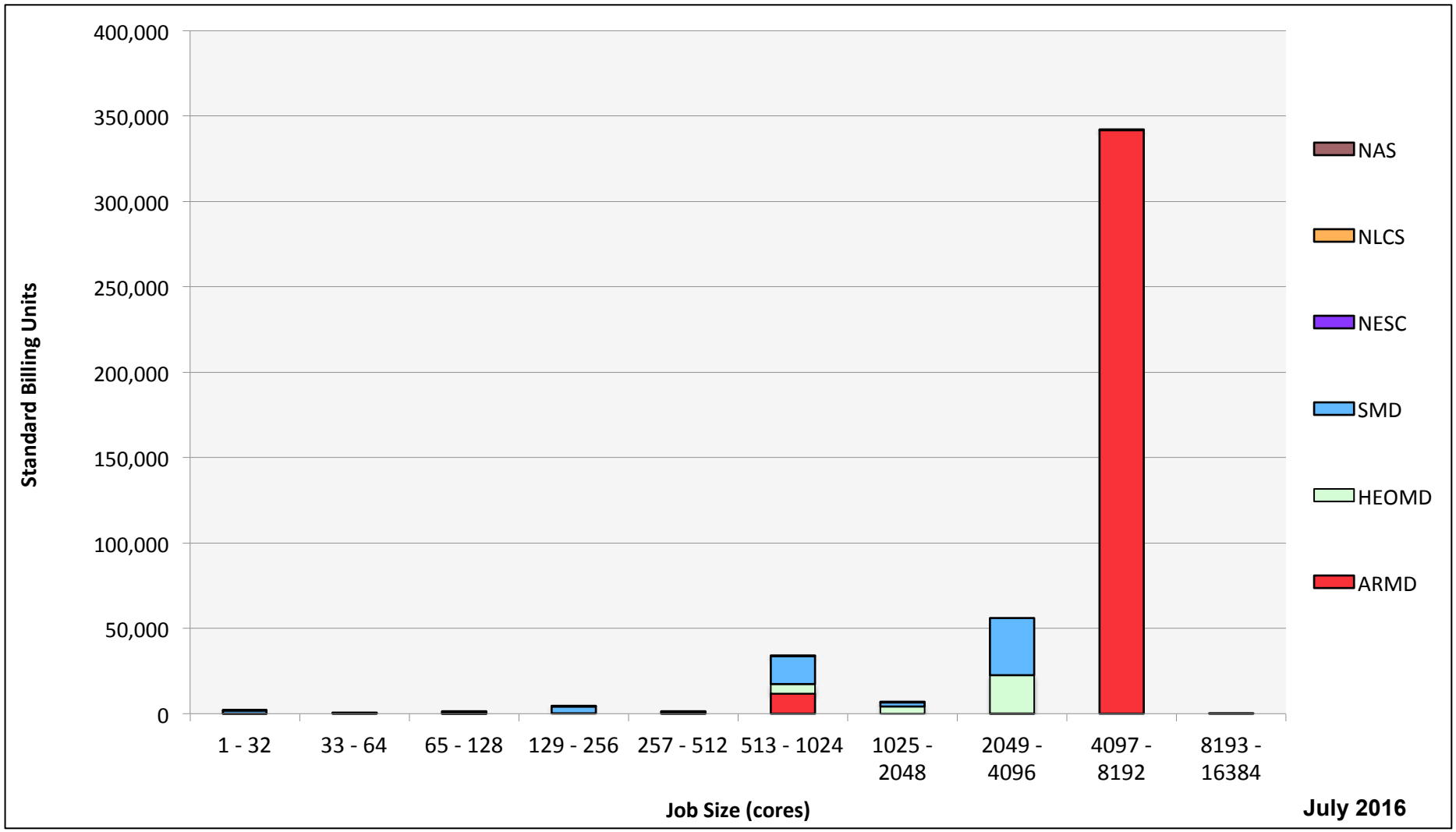
Merope:
SBUs Reported, Normalized to 30-Day Month



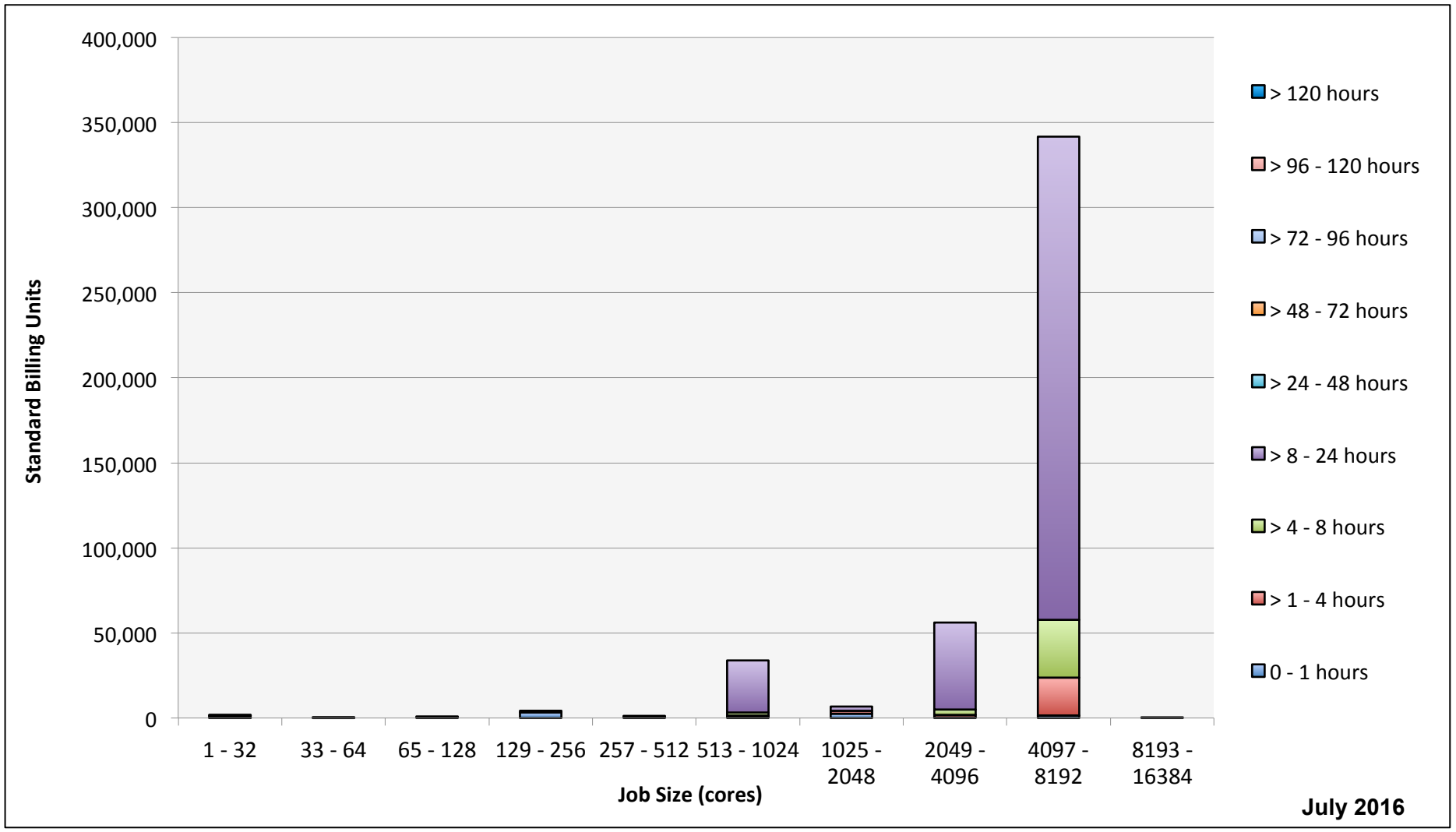
Merope:
Monthly Utilization by Job Length



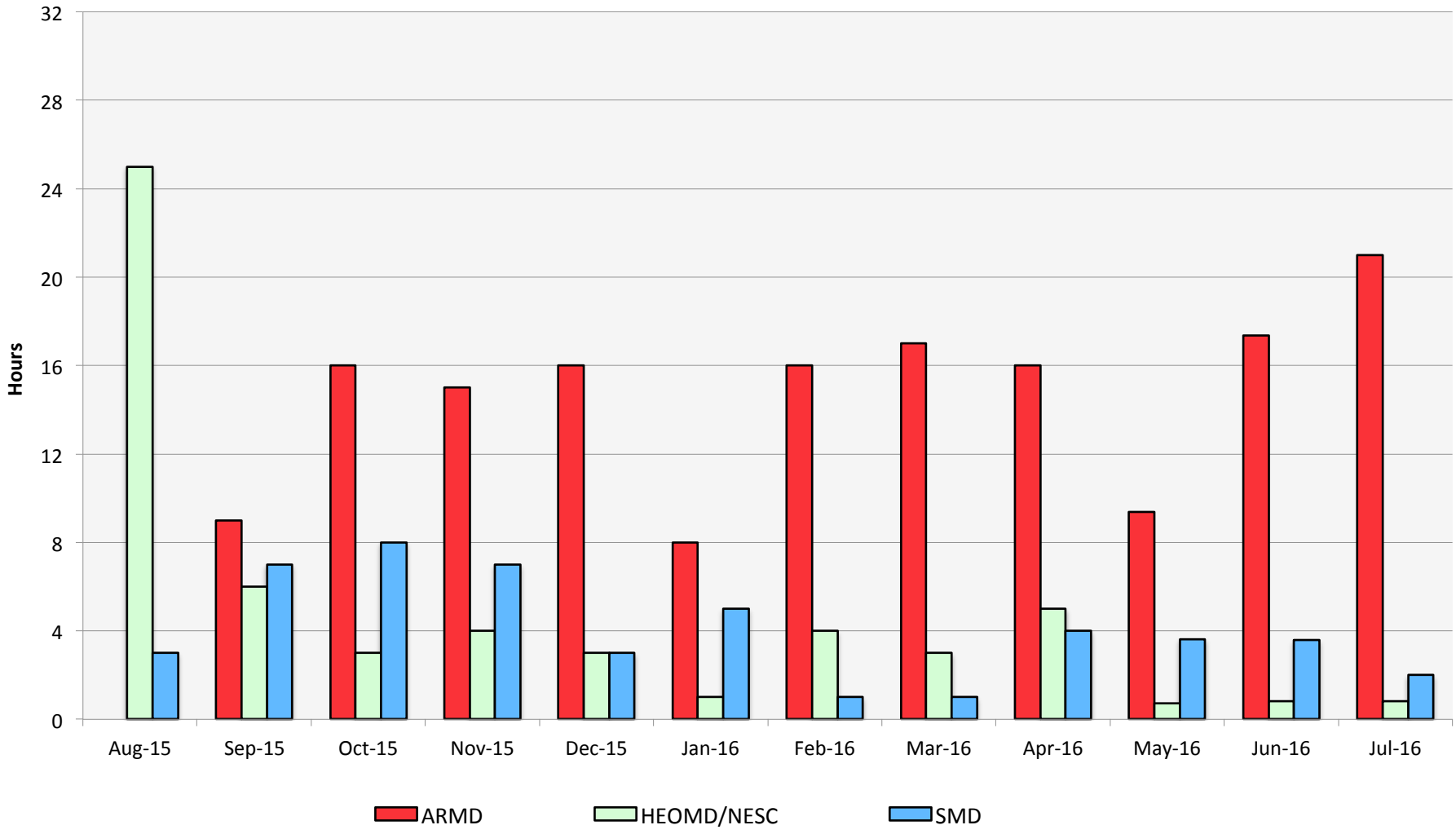
Merope:
Monthly Utilization by Size and Mission



Merope:
Monthly Utilization by Size and Length



Merope:
Average Time to Clear All Jobs



Merope:
Average Expansion Factor