Project Status Report

High End Computing Capability
Strategic Capabilities Assets Program

June 10, 2016

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New Cooling Tower Installed to Improve Supercomputer Reliability and Uptime

- As the culmination of a multi-year project, the HECC Facilities team oversaw a successful cutover to the new cooling tower May 14–17.
- The new cooling tower's spare pump (four-cell design) allows for maintenance without having to shut down the supercomputing systems to clean it, and will allow the chillers that serve Pleiades to maintain cooling capacity throughout the summer, eliminating the decline that occurred on hot summer days with the old tower.
- The new tower's performance specifications include:
  - Total heat rejection capacity of 12 megawatts.
  - Improved water flow to all four chillers from 5,200 gallons per minute (GPM) to 8,400 GPM.
  - Keeps water 7 degrees Fahrenheit cooler on high web-bulb (hot) days than with the old tower.
- HECC facilities engineers coordinated with NASA Ames' Code J engineers and contractor DPR/Turner to connect the tower. Many months of planning and logistics work helped ensure a smooth transition to the new system.
- Installation of the new cooling tower positions the NAS facility to increase cooling capacity for NASA's heavily used supercomputing resources for many years.

Mission Impact: The new cooling tower, with a four-cell design, will provide consistent cooling capacity to the Pleiades supercomputer, yielding a higher level of computer uptime for HECC users.

The newly completed cooling tower is located adjacent to the NASA Advanced Supercomputing facility. Piping provides water to each of four cells, which can be isolated from one another to maintain tower operation during maintenance activities or during single-cell failures.

POCs: John Parks, john.w.parks@nasa.gov, (650) 604-4225, Mark Tangney, mark.l.tangney@nasa.gov, (650) 604-4415, NASA Advanced Supercomputing Division

Facilities Engineers Complete Building Maintenance During Cooling Tower Cutover

- HECC facilities engineers conducted maintenance on building N258 key infrastructure elements in tandem with the new cooling tower cutover (see slide 2).
- The team performed the following critical maintenance on the electrical distribution network:
  - Installed new protection relays throughout the N258 sub-station.
  - Replaced current transformers on the Rotary Uninterruptible Power Supply (RUPS) output breaker. The electrical maintenance addressed infrastructure problems that caused N258 power outages in October and November 2015.
  - Moved power supply for the main N258 communications room to the distribution switch that will provide RUPS protection.
  - Cleaned the four 450-ton chiller condenser tubes and the computer room air handlers, to support the new cooling tower.
- HECC engineers coordinated with NASA Ames Code J/ Jacobs Engineering to restore building power and communications in just over 24 hours. They also provided building support to keep critical infrastructure up until cooling was restored.
- Additional activities included cleaning the sub-floor of the main computer room, installing new carpet in the Control Room, and testing all fire alarms.

Mission Impact: The NASA Advanced Supercomputing (NAS) facility houses the largest high-end computing resource for NASA and, as such, is an extremely important building to keep running at peak efficiency. Proactively identifying and maintaining the power, cooling, network, and compute hardware greatly reduces the risk of building failures.

New relays installed with a dedicated battery UPS provide the NAS facility electrical system with modern overcurrent protection that will help eliminate outages caused by infrastructure failure.

POCs: John Parks, john.w.parks@nasa.gov, (650) 604-4225, Mark Tangney, mark.l.tangney@nasa.gov, (650) 604-4415, NASA Advanced Supercomputing Division

System Maintenance Activities Successfully Completed During Facility Shutdown

- During the annual building maintenance (see slide 3), systems engineers successfully completed maintenance activities on HECC resources. The activity was timed to coincide with the facility work to minimize the impact on users.
- Activities completed include:
  - Updated firmware
  - Refreshed infrastructure systems
  - Applied operating system patches and software updates
  - Replaced faulty components
  - Updated the Lustre filesystem
  - Upgraded the cluster management software (see slide 5)
- In addition, the HECC team conducted system regression testing, which included running the HPCG benchmark, along with a NASA-specific set of regression tests to help identify marginal components in the system.

Mission Impact: Regular maintenance on the HECC systems provides a stable and well-performing system for NASA users.

HECC systems maintenance activities coincided with a planned cooling tower cutover and NAS facility building maintenance, which required several days of downtime.

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

Pleiades Infrastructure Software Updated

- During the scheduled system maintenance time (see slide 4), HECC engineers updated the infrastructure software on Pleiades to the latest release SGI Management Center (SMC) to improve maintainability and management of the cluster.
- New features include the ability to easily upgrade infrastructure systems used for cluster management, improved parallel identification of compute nodes and support of the latest release of the operating system. These features result in less time required to update the management software and improved flexibility in the configuration management of the system.
- The HECC team encountered several bugs and worked with SGI engineers in real time to resolve or work around the issues. This close interaction with SGI enabled HECC to quickly resolve complex issues.
- HECC and SGI engineers will have follow up discussions on improving the SMC software to better support NASA's requirements.

Mission Impact: Improving the Pleiades cluster management software results in a more reliable system and reduced downtime for HECC users.

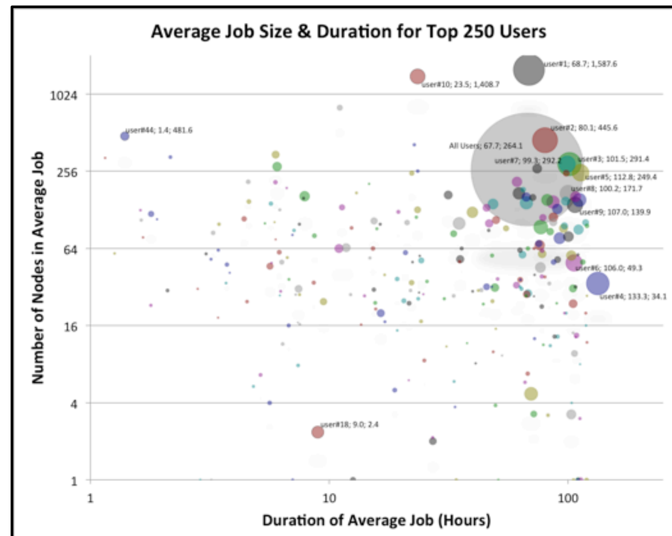
The Pleiades supercomputer was running several administrative systems for the management of the compute nodes that have now been consolidated.

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

APP Team Improves User Experience with Application-Focused Services

- Over the last three months, experts in the HECC Application Performance and Productivity (APP) team provided a diverse set of services to improve users' experiences on HECC resources.
- Much of the team's impact comes from helping users directly. For example, the team:
  - Helped several users who needed changes in complicated build scripts; one needed to combine files from OVERFLOW and FUN3D into a single executable.
  - Helped a user prepare for 20K-, 40K-, and 100K-core runs after the recent return from dedicated time.
  - Assisted high-priority groups by shepherding critical jobs and creating special job queues.
  - Performed an I/O characteristics study for an important application and recommended several changes to speed it up.
- The team also developed a crash reproducer program that speeds the identification of Pleiades nodes experiencing communication issues.
- In collaboration with the Systems team, the APP team has initiated a Lustre focus group to establish and document best practices and minimum expectations for application I/O behavior.

Mission Impact: HECC application services experts enable researchers to better utilize NASA's super-computing resources for their modeling and simulation projects supporting the agency's mission goals.



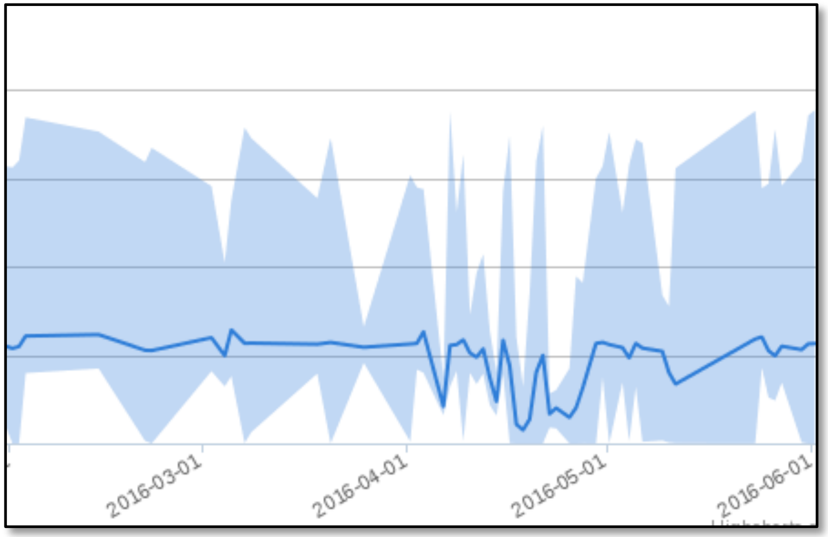
The HECC user community employs varied strategies for accomplishing computational work, and the APP team provides a broad range of services to help them. This graph shows the diversity in user job workloads. Each of the top 250 users is shown as a bubble whose position indicates the user's average job size and average job duration. The area of the bubble is proportional to the amount of compute resources consumed by the user's workload. (**See slide 39 for full scale.**)

POC: Robert Hood, robert.hood@nasa.gov, (650) 604-0740, NASA Advanced Supercomputing Division, CSRA LLC

Network Engineers Work with JPL to Restore Transfer Rates Between Sites

- HECC network engineers collaborated with system administrators at NASA's Jet Propulsion Laboratory (JPL) to identify the root cause of a 50% performance drop in file transfer rates between the NAS facility and JPL.
- The HECC team set up memory-to-memory throughput testing across several JPL servers to identify the source of the problem, and found that the JPL access switches were dropping packets.
- Additionally, they wrote a script to allow JPL systems administrators to monitor network interface utilization on their servers.
  - Using this approach, the HECC team identified that switches were consistently at 99% utilization due to a recent configuration change at JPL that allowed storage area network (SAN) traffic to traverse the same interface, resulting in over-subscribed switches.
- Normal rates were restored when the affected JPL servers were moved to another switch. In addition, JPL is working on another method of handling SAN traffic to avoid competing with wide area network traffic.
- By proactively identifying the source of network problems and collaborating with JPL administrators, our network engineers were able to quickly resolve this issue.

Mission Impact: By taking responsibility for managing network problems end-to-end, HECC network engineers are able to ensure users are provided optimal network performance.



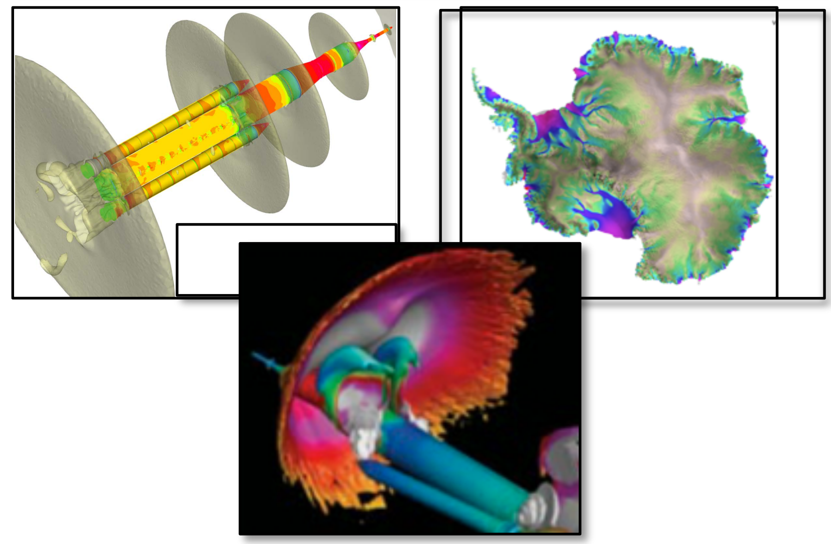
This graph shows the average per-stream transfer (dark blue line) between JPL and the NAS facility from February to June 2016. Each horizontal line in the graph represents 100 megabits per second (Mbps); rates between the two centers dipped from 220 Mbps to as low as 110 Mbps in April.

POCs: Nichole Boscia, nichole.k.boscia@nasa.gov, (650) 604-0891, Chris Buchanan, chris.buchanan@nasa.gov, (650) 604-4308, NASA Advanced Supercomputing Division, CSRA LLC

New Allocation Period for Supercomputing Time Begins for NASA Mission Directorates

- May 1, 2016 marked the beginning of a new allocation period for the Human Exploration and Operations Mission Directorate (HEOMD), the NASA Engineering and Safety Center (NESC), and about half of the Science Mission Directorate (SMD).
- These organizations awarded allocations of computing time on Pleiades and Endeavour to 220 computing projects.
- Requests for time from HEOMD and NESC were 135% of available time, and requests for time from SMD were over 300% of available time.
- Combined awards were approximately 70 million Standard Billing Units* (SBUs) for the six-month allocation period.
- The new allocation period is an opportunity for each organization to assess demands for computing time and to rebalance allocations to meet computing needs for the next year.

Mission Impact: NASA programs and projects periodically review the distribution of supercomputer time to assess the demand for resources and assure consistency with mission-specific goals and objectives.



Representative images of NESC, SMD, and HEOMD projects supported by HECC resources. Clockwise from left: 1) Surface pressure coefficient with sonic isosurfaces from an 11,640-processor computation of the transonic flow about a Space Launch System configuration, *S. Alter, NASA/Langley.* 2) Computed ice surface velocities for Antarctica, *G. Perez, U.C. Irvine, Eric Larour, NASA/JPL.* 3) Space Launch System booster separation flow field, *S. Rogers, NASA Ames; R. Rocha, U.C. Davis.*

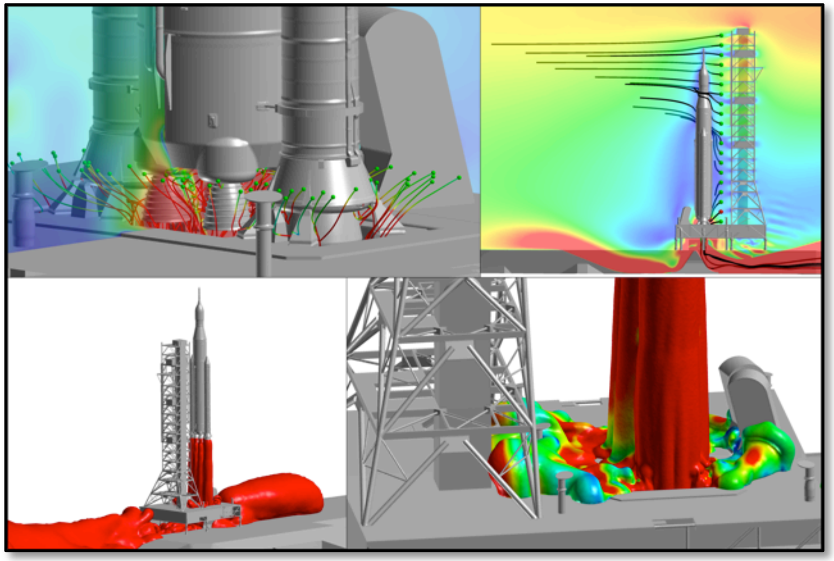
POC: Catherine Schulbach, catherine.h.schulbach@nasa.gov, (650) 604-3180, NASA Advanced Supercomputing Division

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

Analyzing the Space Launch System Debris Environment *

- Researchers at NASA Marshall ran high-fidelity computational fluid dynamics (CFD) simulations on Pleiades to help Space Launch System (SLS) designers understand all expected sources of debris and the impact energy the debris may impart to the launch vehicle.
  - The simulations reveal the fluid flow features (such as ignition overpressure, and plume impingement and recirculation on launch platform surfaces) that may act as transport mechanisms for debris.
  - The resulting data was coupled with models of typical debris to predict trajectories and identify the affected components of the vehicle.
- Analyses included:
  - Static CFD simulations of the vehicle on the launch pad representing the flow conditions that debris may experience prior to liftoff.
  - A time-accurate CFD simulation of the vehicle's ignition transient and motion along a launch trajectory for the first few seconds of flight.
- The simulations help designers ensure each SLS component can survive debris impacts (or eliminate sources of debris) so the vehicle can launch safely.

Mission Impact: Enabled by HECC resources, these simulations reduced the uncertainty and conservatism of earlier debris environment analyses and led to an updated debris environment that was key to the successful completion of the SLS Critical Design Review.



Visualizations showing computational fluid dynamics simulations of the Space Launch System vehicle on the launch pad. Isosurfaces of velocity (colored red to blue) and streamlines from the simulations illustrate the flow fields that act as transport mechanisms for liftoff debris.

***POC**:* Brandon Williams, brandon.williams@nasa.gov, (256) 544-3637, NASA Marshall Space Flight Center, Jacobs ESSSA Group

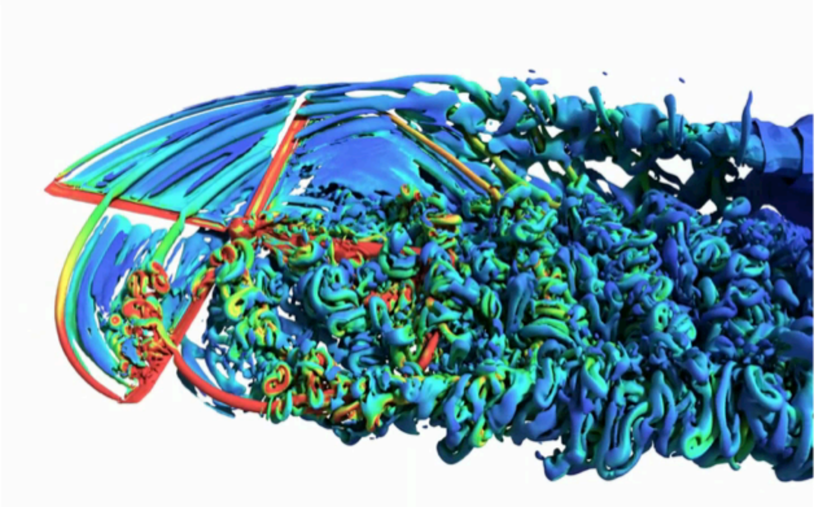
** HECC provided supercomputing resources and services in support of this work*

Improved Resolution of Rotorcraft Flows Using AMR Method *

- To support NASA's Revolutionary Vertical Lift Technology (RVTL) project, researchers at NASA Ames ran state-of-the-art rotorcraft simulations on Pleiades to improve vehicle designs and reduce noise levels created by blade-vortex interaction (BVI) and dynamic stall.
- The RVLT project used AMR to:
  - For the first time, apply near-body adaptive mesh refinement (AMR) methods to flexible rotors in forward flight using the OVERFLOW Navier-Stokes CFD code.
  - Demonstrate improved spatial resolution for BVI and dynamic stall phenomena; the latter limits rotorcraft flight speed in forward flight.
  - Verify whether discrepancies between computation and experiment are due to deficiencies in aerodynamic resolution or deficiencies in the structural model of a flexible rotor blade.
- Additional computations will be carried out on Pleiades to quantify and validate the AMR approach with experimental measurements.

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

Mission Impact: Enabled by Pleiades, high-resolution, near body AMR simulations and animations of unsteady rotorcraft flow provide a better understanding of complex flow phenomena and improve the accuracy of sound level and aerodynamic loads prediction due to BVI and dynamic stall.



The vortex wake generated by a spinning rotor as it advances into a headwind at high speed. As the blade retreats from the headwind, the flow separates along the blade and forms detached vortex rings that move downwind, causing a loss of lift and a nose-down pitching moment that limits the vehicle's flight speed. The flow is colored by vorticity magnitude: red is high and blue is low. *Tim Sandstrom, NASA/Ames*

POC: Neal Chaderjian, neal.chaderjian@nasa.gov, (650) 604-4472, NASA Advanced Supercomputing Division

HECC Facility Hosts Several Visitors and Tours in May 2016

- HECC hosted 6 tour groups in May; 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 scheduled facility maintenance. Visitors this month included:
  - Undergrad students from the Blue Marble Space Institute of Science, Young Scientist Program.
  - A group from the Dwight D. Eisenhower School for National Security and Resource Strategy at the National Defense University campus.
  - Rajiv Kumar Tayal, Executive Director for the Indo-US Science Technology Forum (IUSSTF) located in New Delhi, India.
  - Pal Brekke, an Earth scientist and filmmaker, who presented his film, “The Northern Lights,” at the NASA Ames Directors Colloquium.

Visitors to the NASA Advanced Supercomputing facility are typically given a tour through the main computer room housing the Pleiades supercomputer and the mass storage archive (shown above), which was recently expanded to three times its previous capacity.

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

Papers

- "**Mass Transport and Turbulence in Gravitationally Unstable Disk Galaxies II: The Effects of Star Formation Feedback**," J. Goldbaum, M. Krumholz, J. Forbes, arXiv: 1605.00646 [astro-ph.GA], May 2, 2016. *
http://arxiv.org/abs/1605.00646
- "**An Approach to Computing Discrete Adjoints for MPI-Parallelized Models Applied to the Ice Sheet System Model**," E. Larour, J. Utke, A. Bovin, M. Morlighem, G. Perez, Geoscientific Model Development: Discussions, May 9, 2016. *
http://www.geosci-model-dev-discuss.net/gmd-2016-99
- "**Radiative, Two-Temperature Simulations of Low Luminosity Black Hole Accretion Flows in General Relativity**," A. Sadowski, M. Wielgus, R. Narayan, D. Abarca, J. McKinney, arXiv:1605.03184 [astro-ph.HE], May 10, 2016. *
http://arxiv.org/abs/1605.03184
- "**DISCO: A 3D Moving-Mesh Magnetohydrodynamics Code Designed for the Study of Astrophysical Disks**," P. Duffell, arXiv:1605.03577 [physics.comp-ph], May 11, 2016. *
http://arxiv.org/abs/1605.03577
- "**Data Constrained Coronal Mass Ejections in a Global Magnetohydrodynamics Model**," M. Jin, et al., arXiv:1605.05360 [astro-ph.SR], May 17, 2016. *
http://arxiv.org/abs/1605.05360

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

Papers (cont.)

- "**Computational Framework for Launch, Ascent, and Vehicle Aerodynamics (LAVA)**," C. Kiris, J. Housman, M. Barad, E. Sozer, C. Brehm, S. Moini-Yekta, Aerospace Science and Technology (accepted article), May 26, 2016. *
  http://www.sciencedirect.com/science/article/pii/S127096381630178X
- **AIAA/CEAS Aeroacoustics Conference**, Lyon, France, May 30–June 1, 2016
  - "**Simulation-Based Airframe Noise Prediction of a Full-Scale, Full Aircraft**," M. Khorrami, E. Fares. *
    http://arc.aiaa.org/doi/abs/10.2514/6.2016-2706
  - "**Airframe Noise Prediction of a Full Aircraft in Model and Full Scale Using a Lattice Boltzmann Approach**," E. Fares, B. Duda, M. Khorrami. *
    http://arc.aiaa.org/doi/10.2514/6.2016-2707
  - "**Computational Evaluation of Airframe Noise Reduction Concepts at Full Scale**," M. Khorrami, B. Duda, A. Hazir, E. Fares. *
    http://arc.aiaa.org/doi/10.2514/6.2016-2711

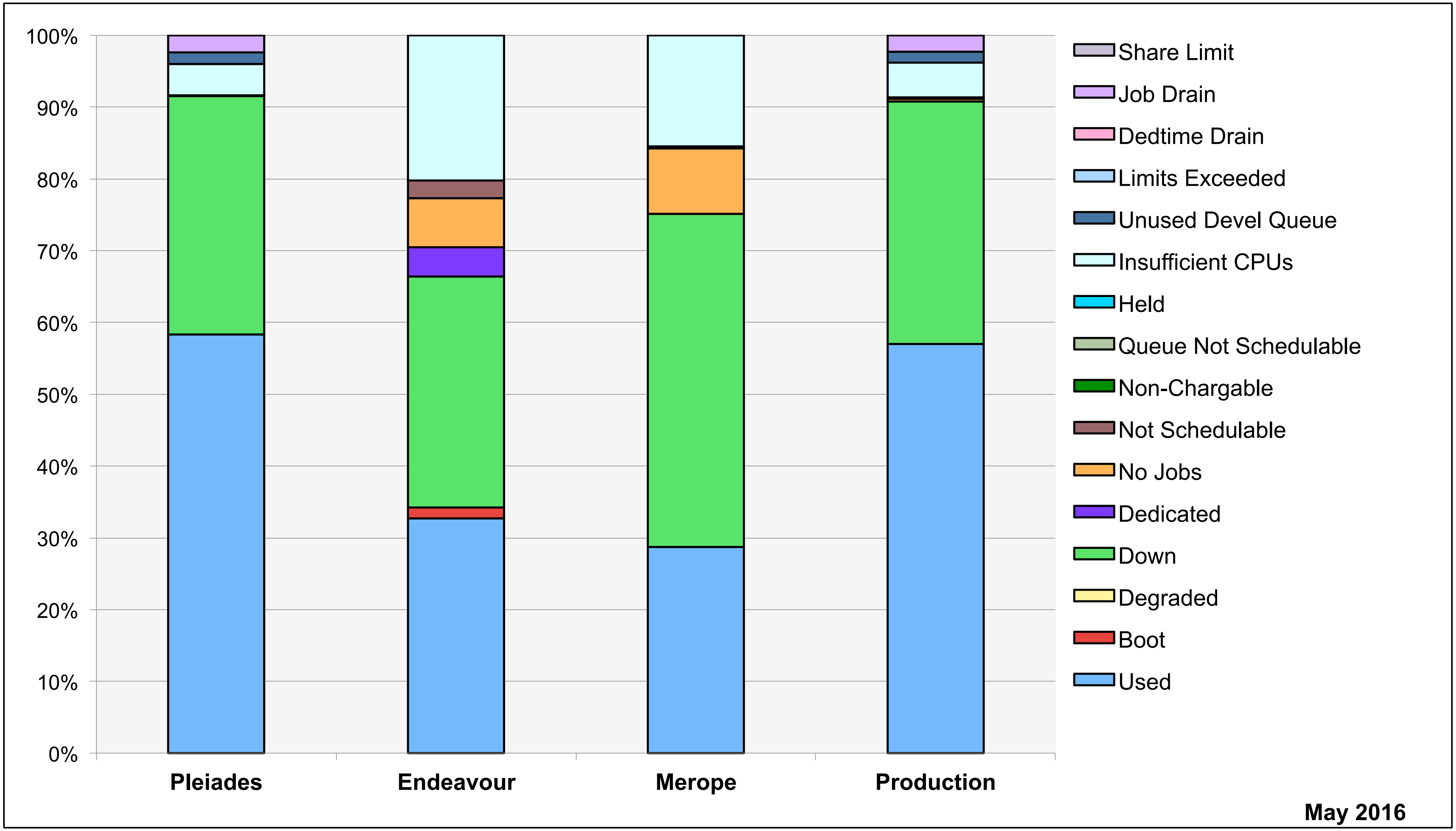
** HECC provided supercomputing resources and services in support of this work*

Presentations

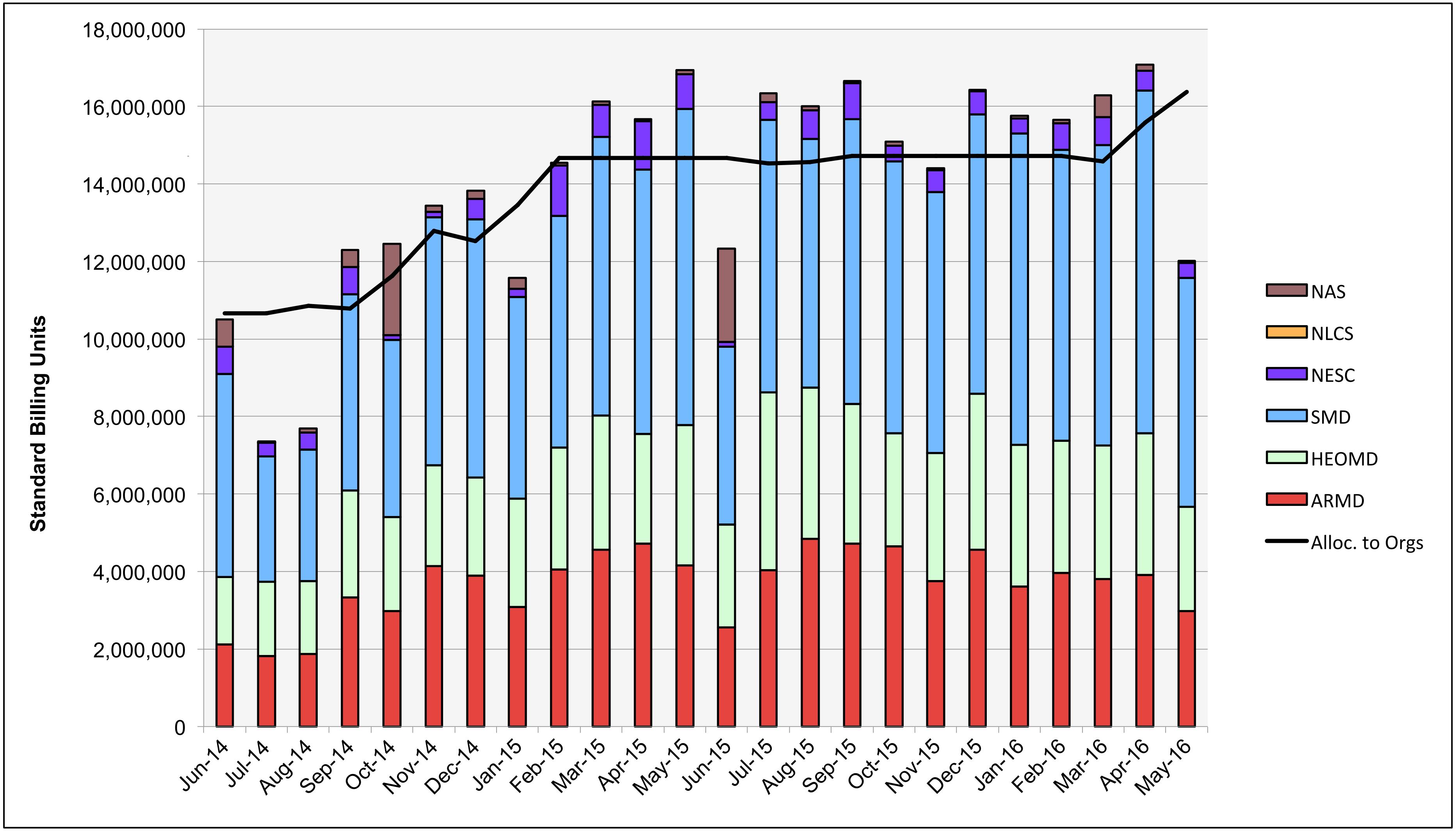
- "**Asteroid Threat Assessment**," D. Mathias, presented at the 35th International Space Development Conference, San Juan, Puerto Rico, May 18–22, 2016. *
- "**Magnetic Flux Emergence and Transport**," N. Mansour, presented at the NASA/NSF Living with a Star TIM at NASA Ames Research Center, May 24–25, 2016. *
- **AIAA/CEAS Aeroacoustics Conference**, Lyon, France, May 30–June 1, 2016.
  - "**Computational Design of a Krueger Flap Targeting Conventional Slat Aerodynamics**," H. D. Akaydin, J. Housman, C. Kiris, C. Bahr, F. Hutcheson. http://arc.aiaa.org/doi/10.2514/6.2016-2958 *
  - "**Slat Noise Predictions using Higher-Order Finite-Difference Methods on Overset Grids**," J. Housman, C. Kiris. http://arc.aiaa.org/doi/pdf/10.2514/6.2016-2963 *
- "**Radiative MHD Simulations of the Formation and Dynamics of Internetwork Magnetic Field and their Effects in the Solar Chromosphere**," I. Kitiashvili, presented at the Solar Physics Division Meeting, Boulder, Colorado, May 31–June 3, 2016. *

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

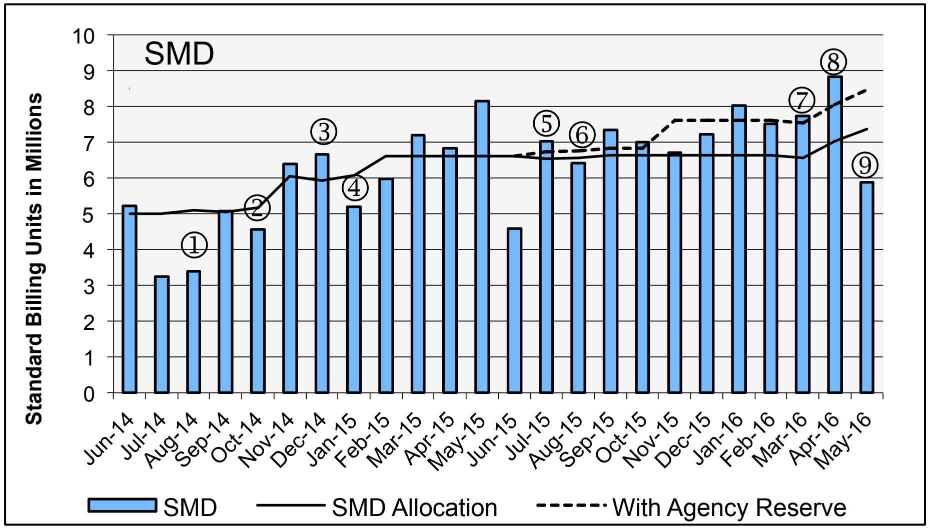
HECC Utilization

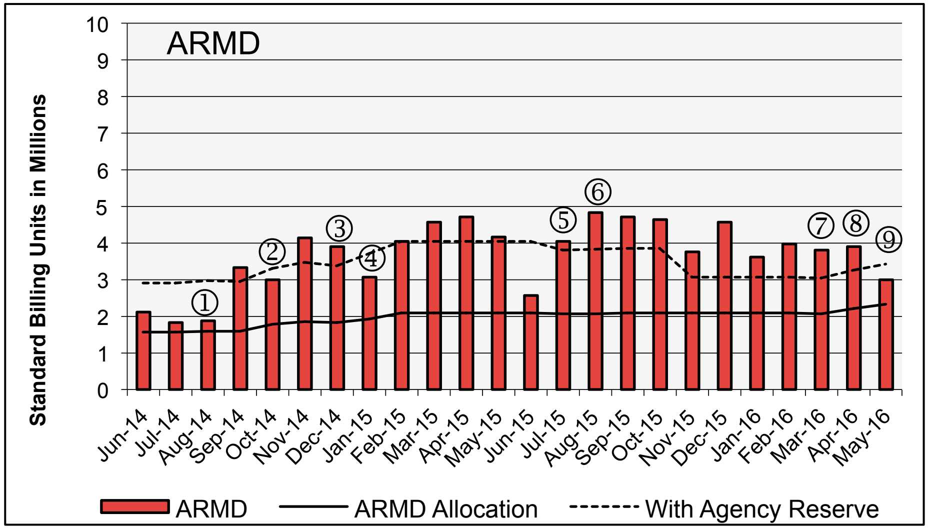


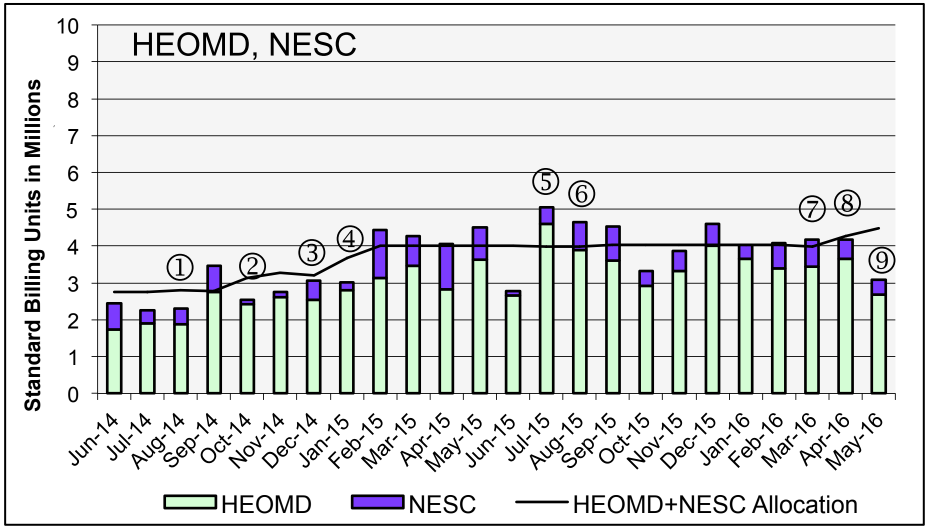
HECC Utilization Normalized to 30-Day Month



HECC Utilization Normalized to 30-Day Month







① 6 Westmere Racks added to Merope, Merope Harpertown retired

② 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

③ 16 Westmere Racks retired from Pleiades

④ 14 Haswell racks added to Pleiades

⑤ 7 Merope Nehalem Racks removed from Merope

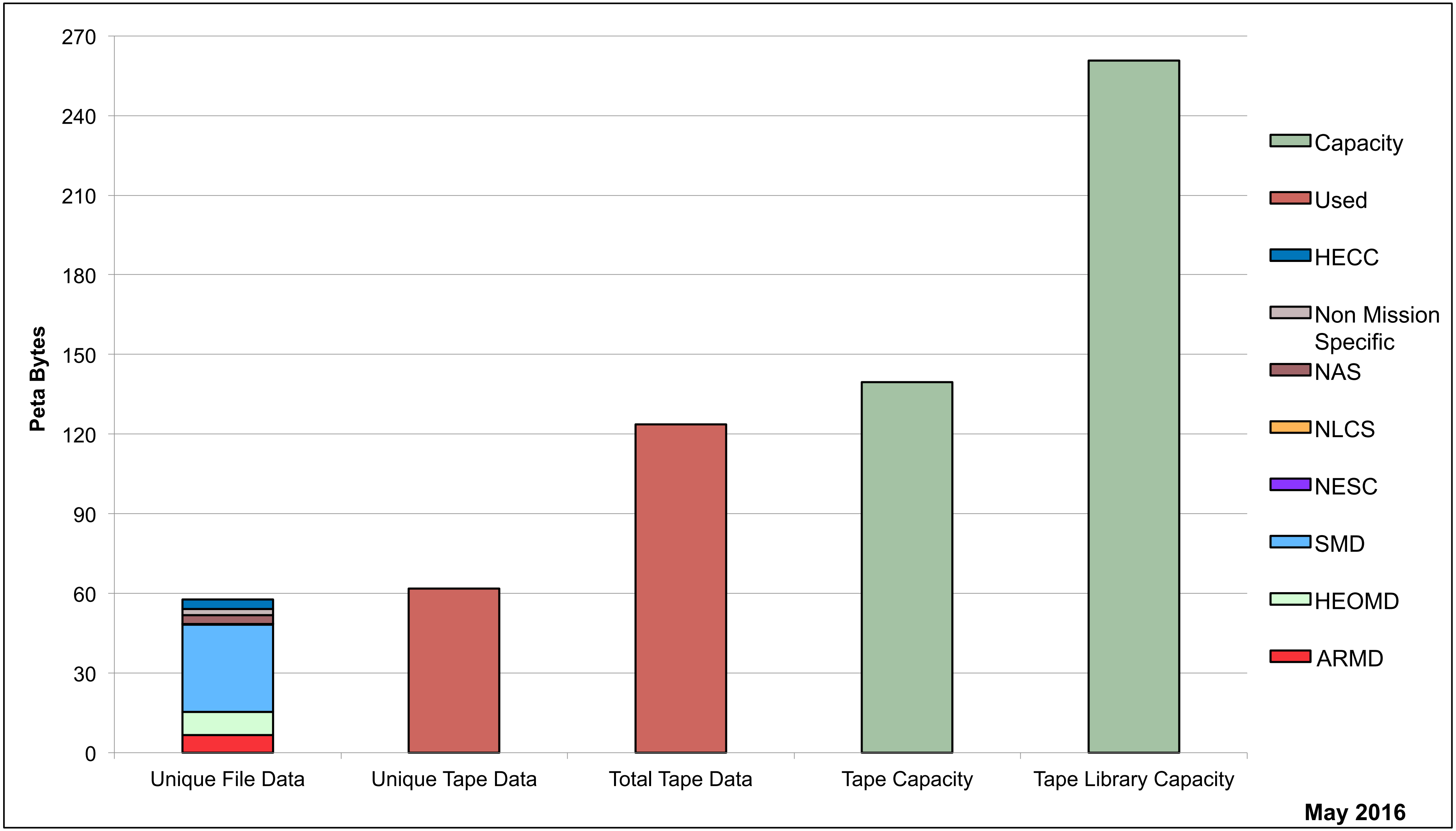
⑥ 7 Merope Westmere Racks added to Merope

⑦ 16 Westmere Racks retired from Pleiades

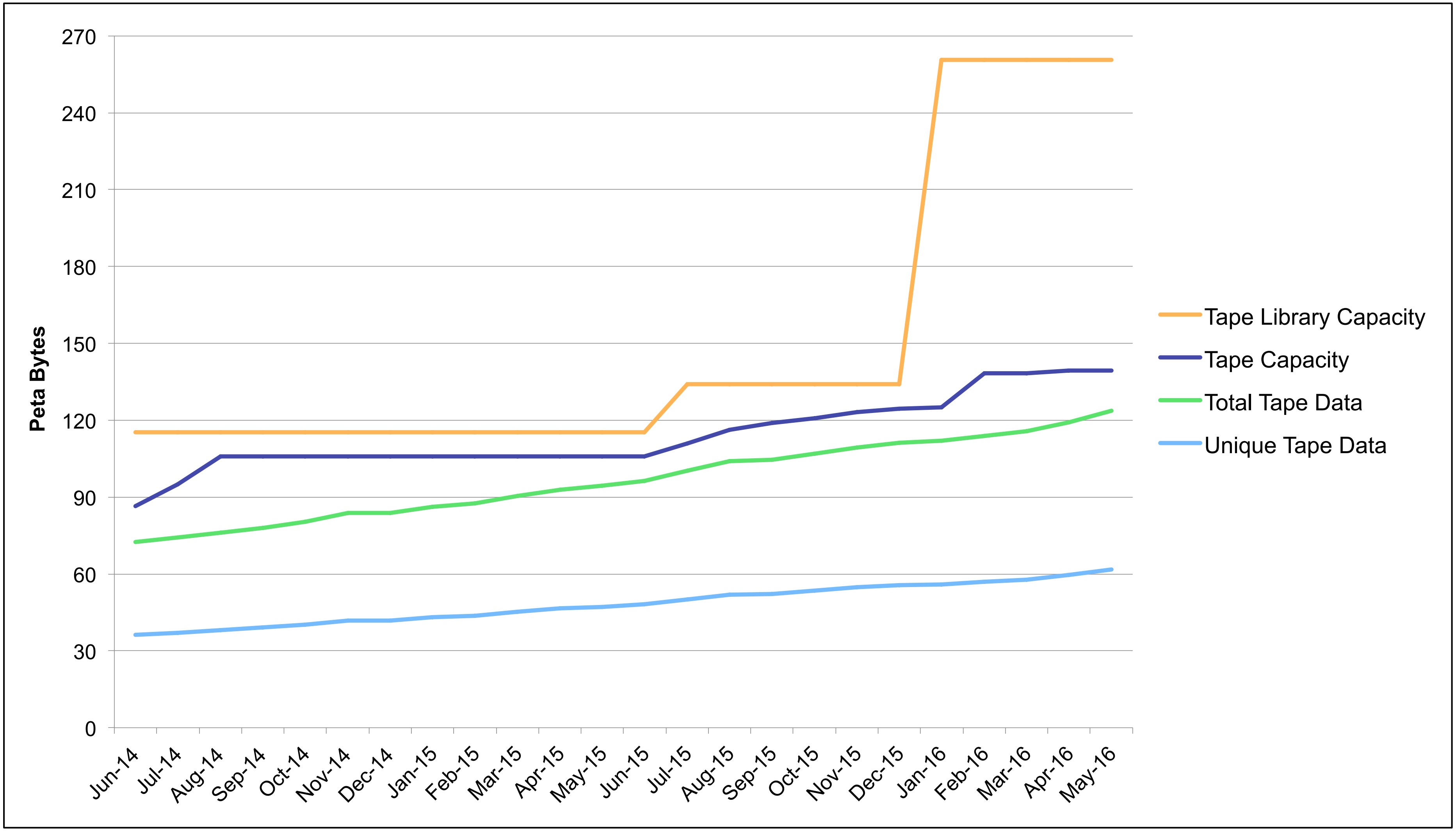
⑧ 10 Broadwell Racks added to Pleiades

⑨ 4 Broadwell Racks added to Pleiades

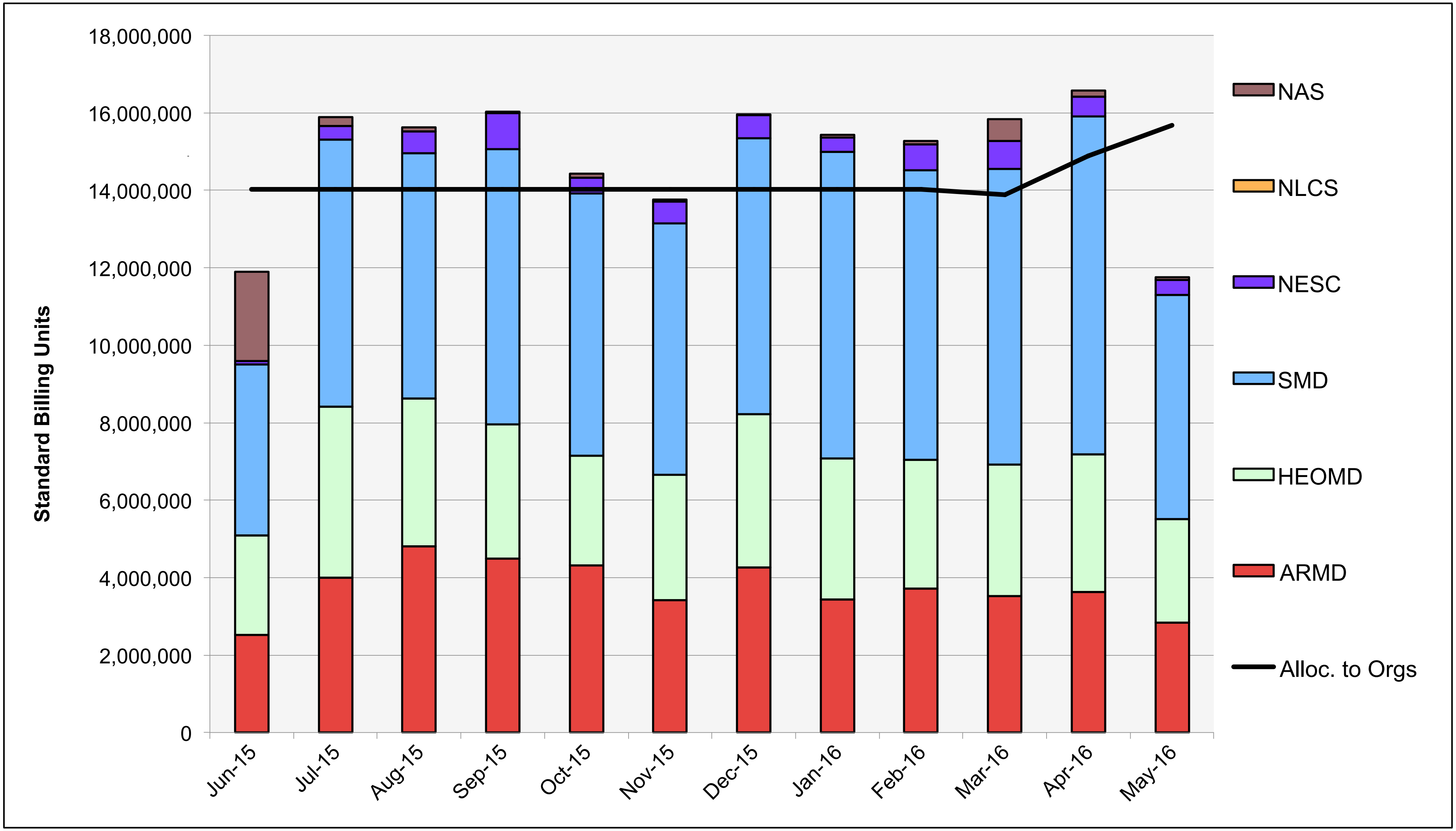
Tape Archive Status



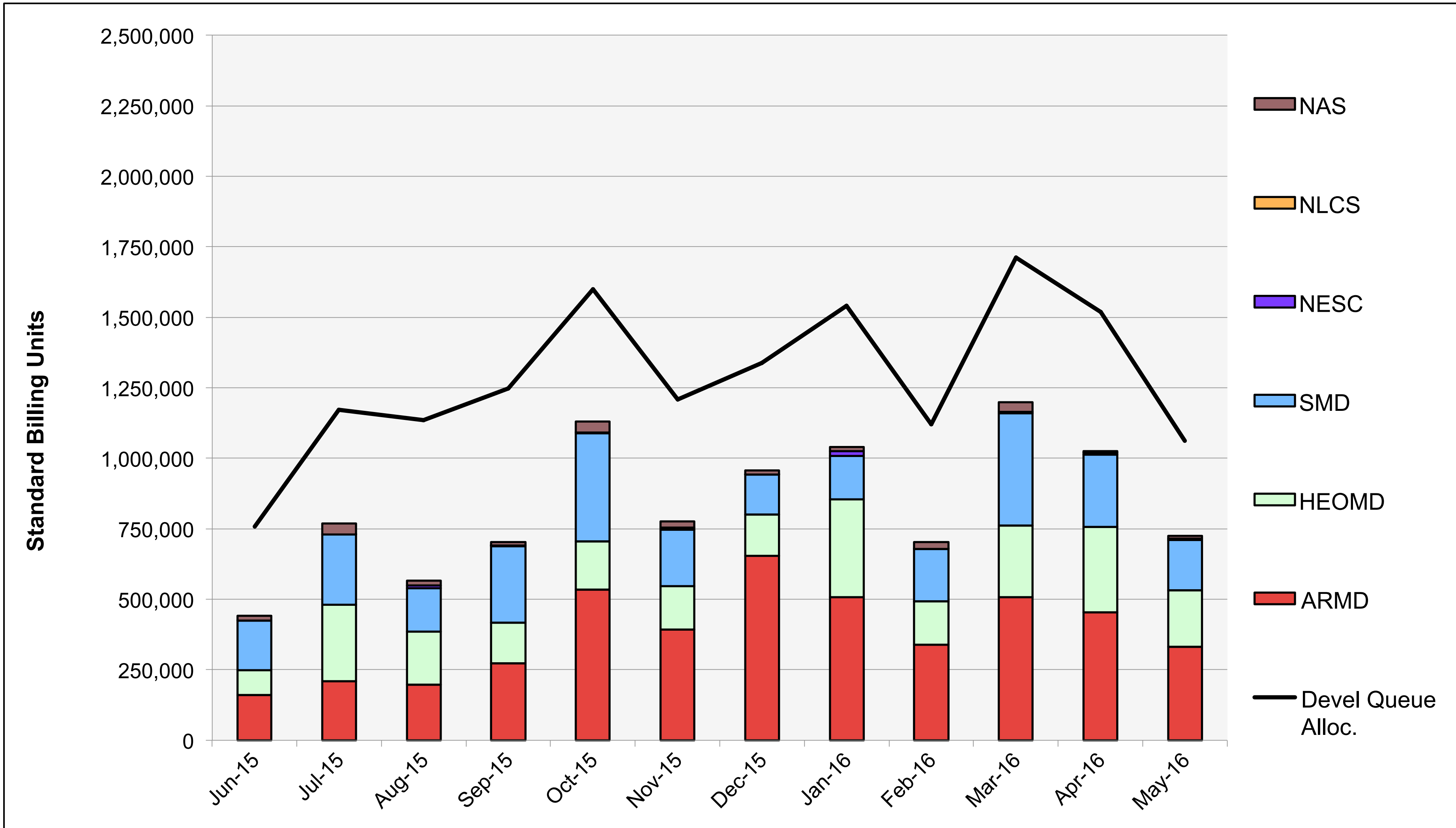
Tape Archive Status



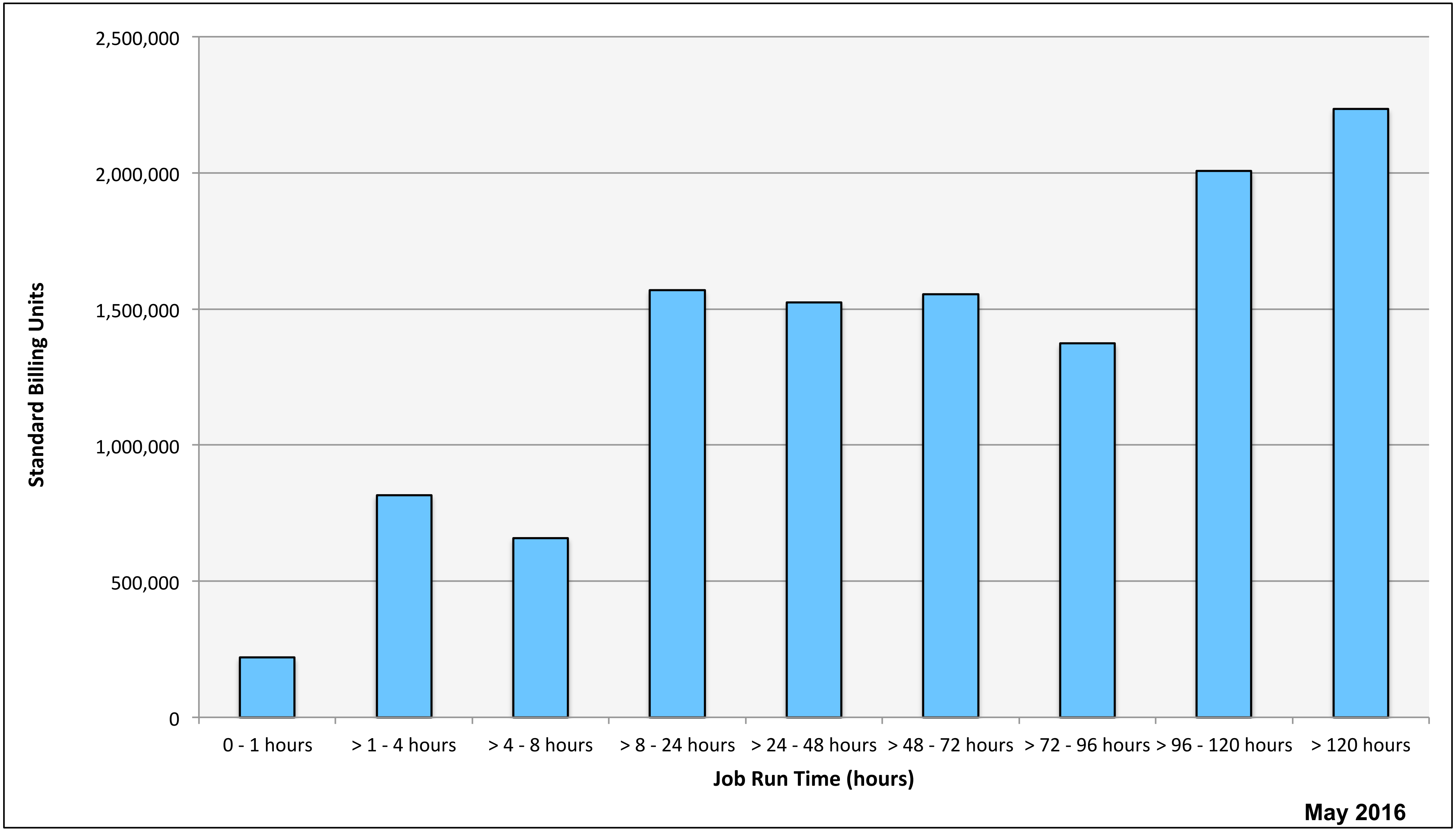
Pleiades:
SBUs Reported, Normalized to 30-Day Month



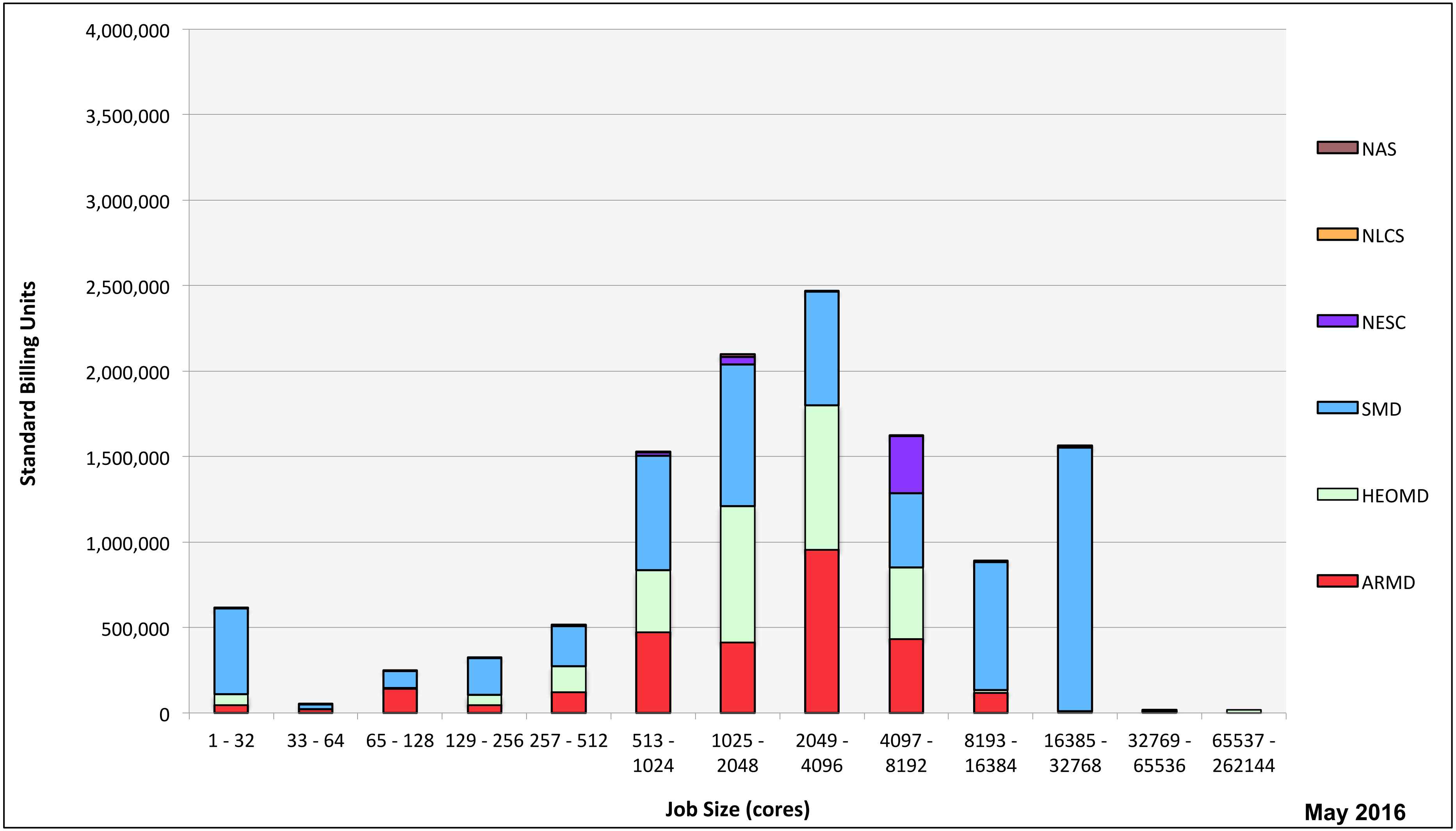
Pleiades: Devel Queue Utilization



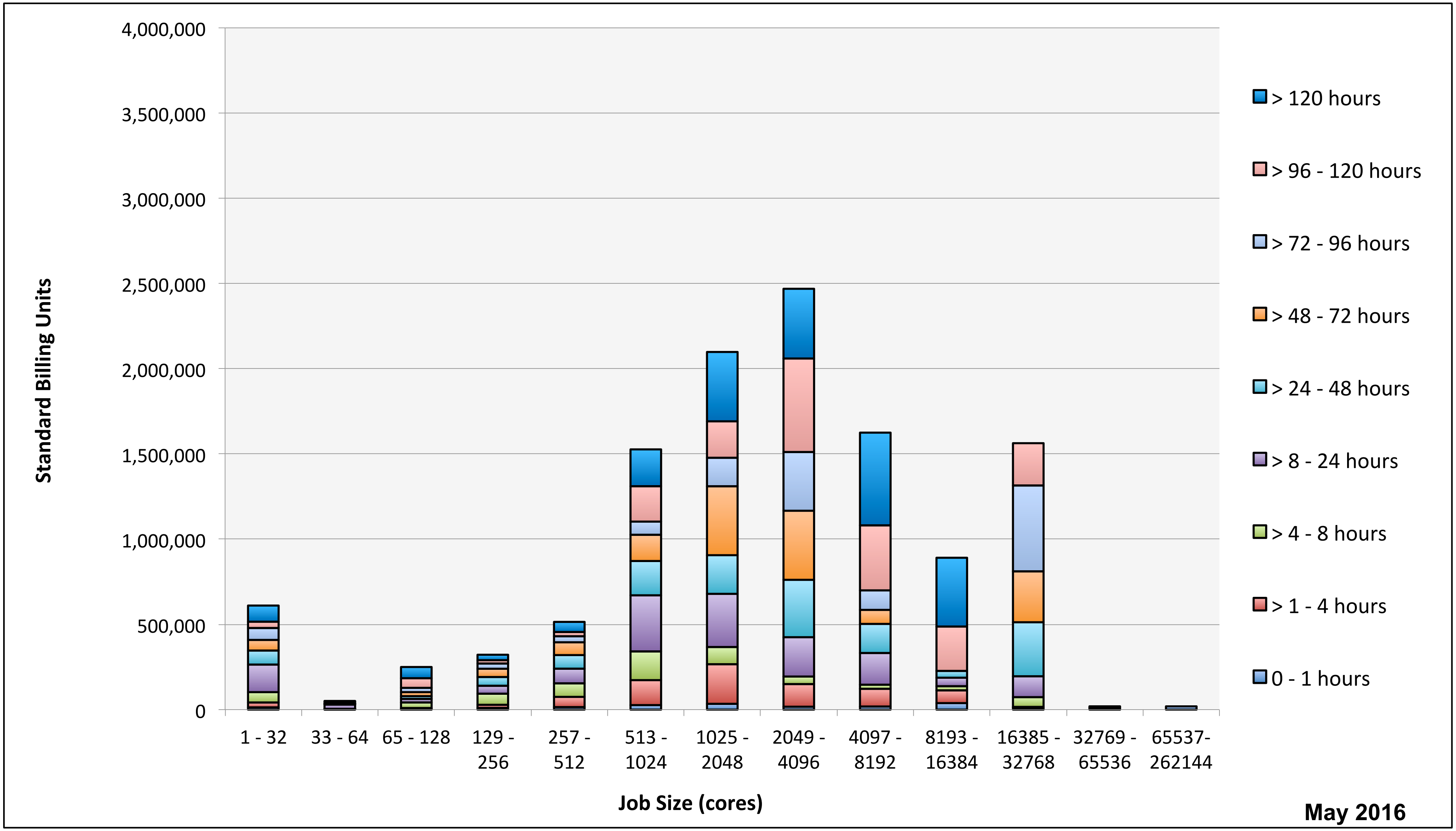
Pleiades:
Monthly Utilization by Job Length



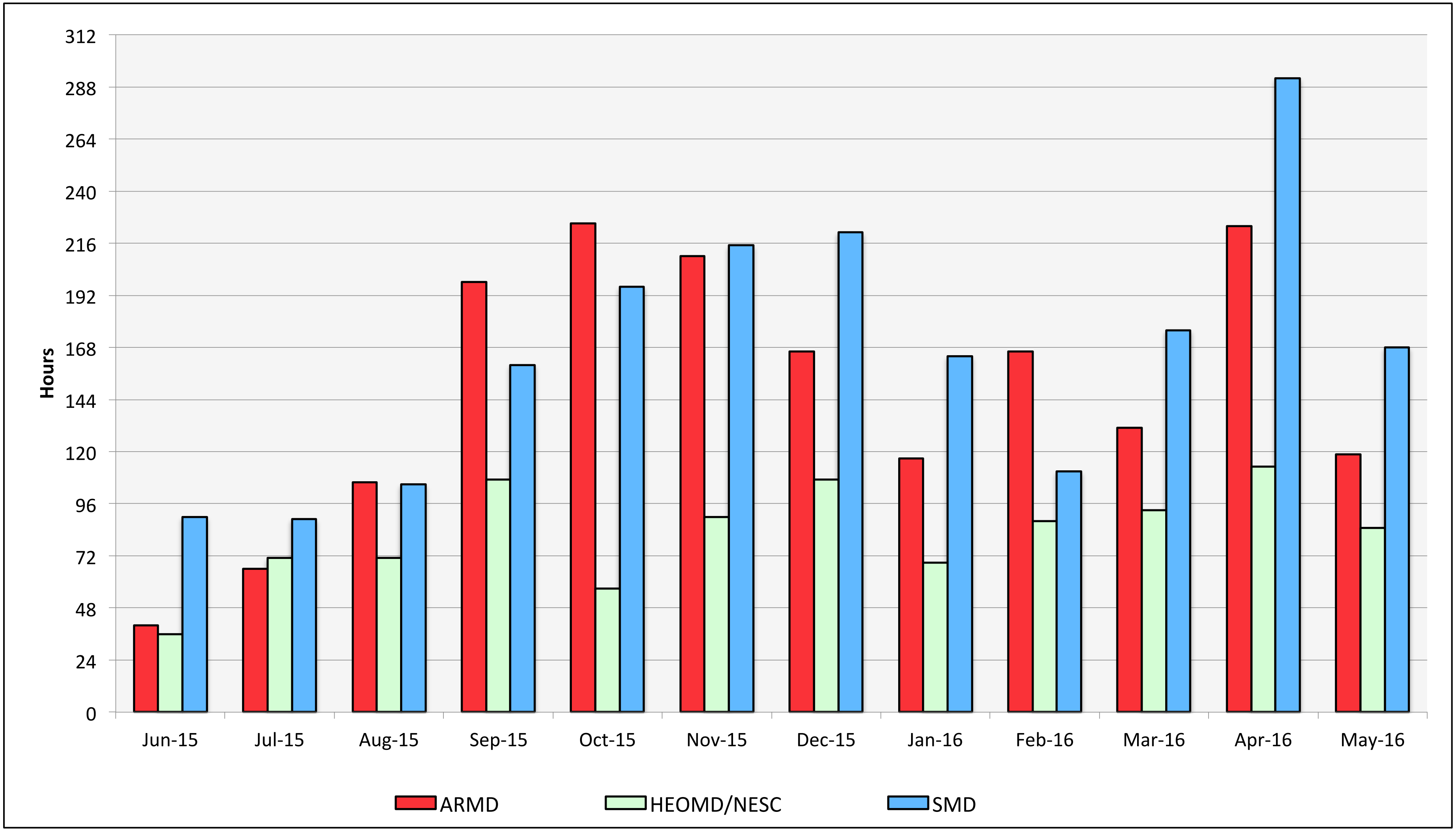
Pleiades: Monthly Utilization by Size and Mission



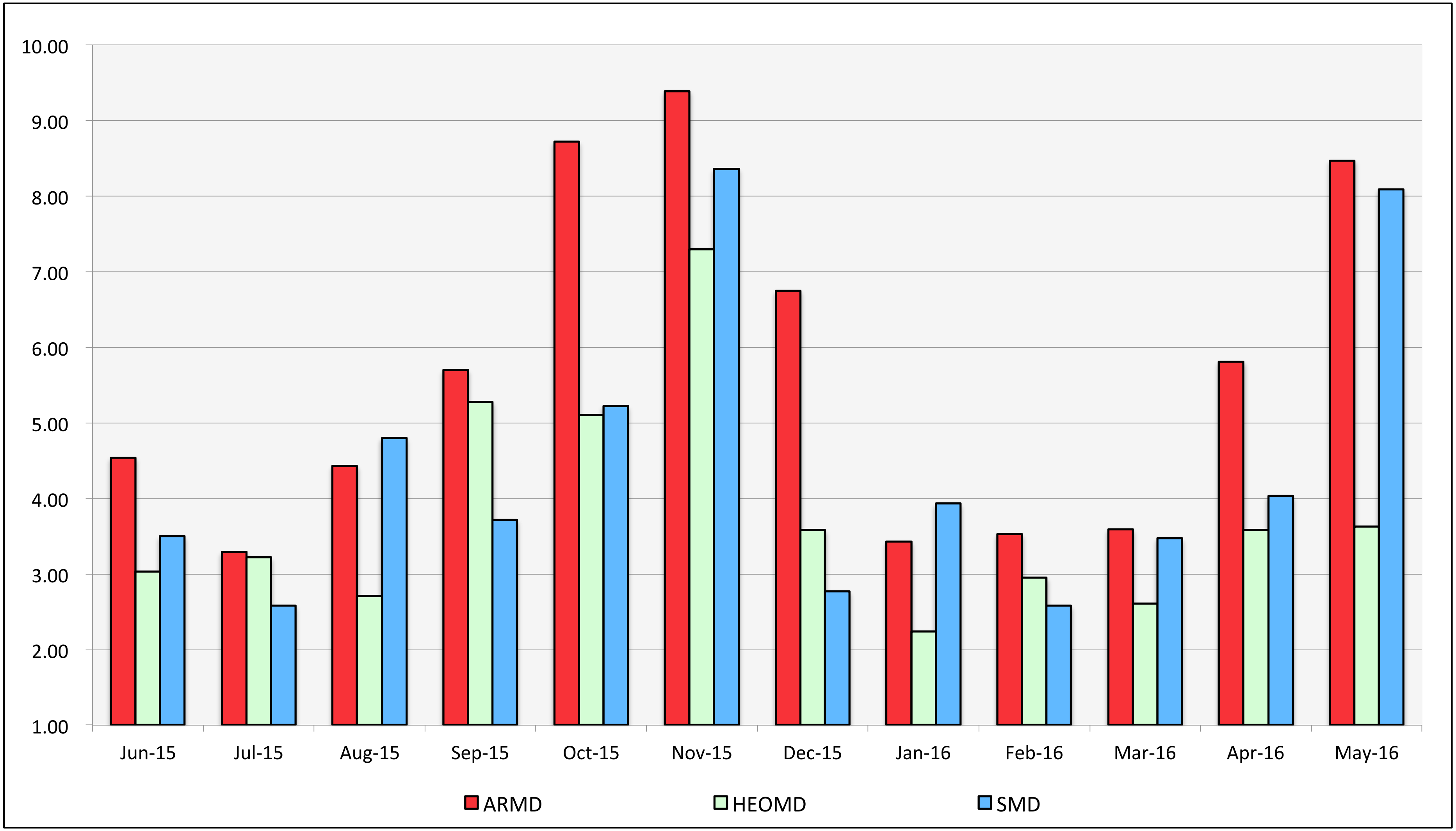
Pleiades:
Monthly Utilization by Size and Length



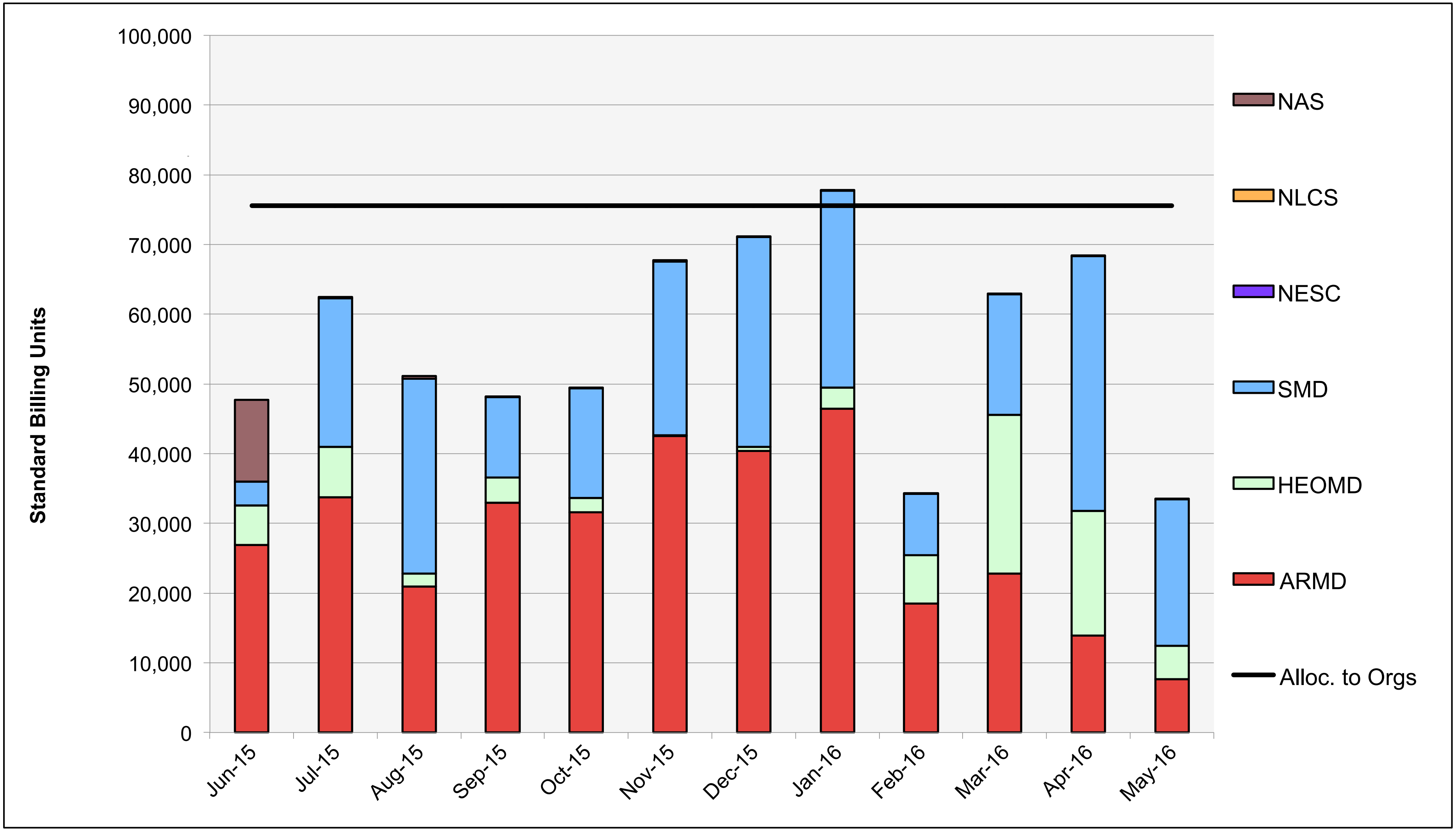
Pleiades: Average Time to Clear All Jobs



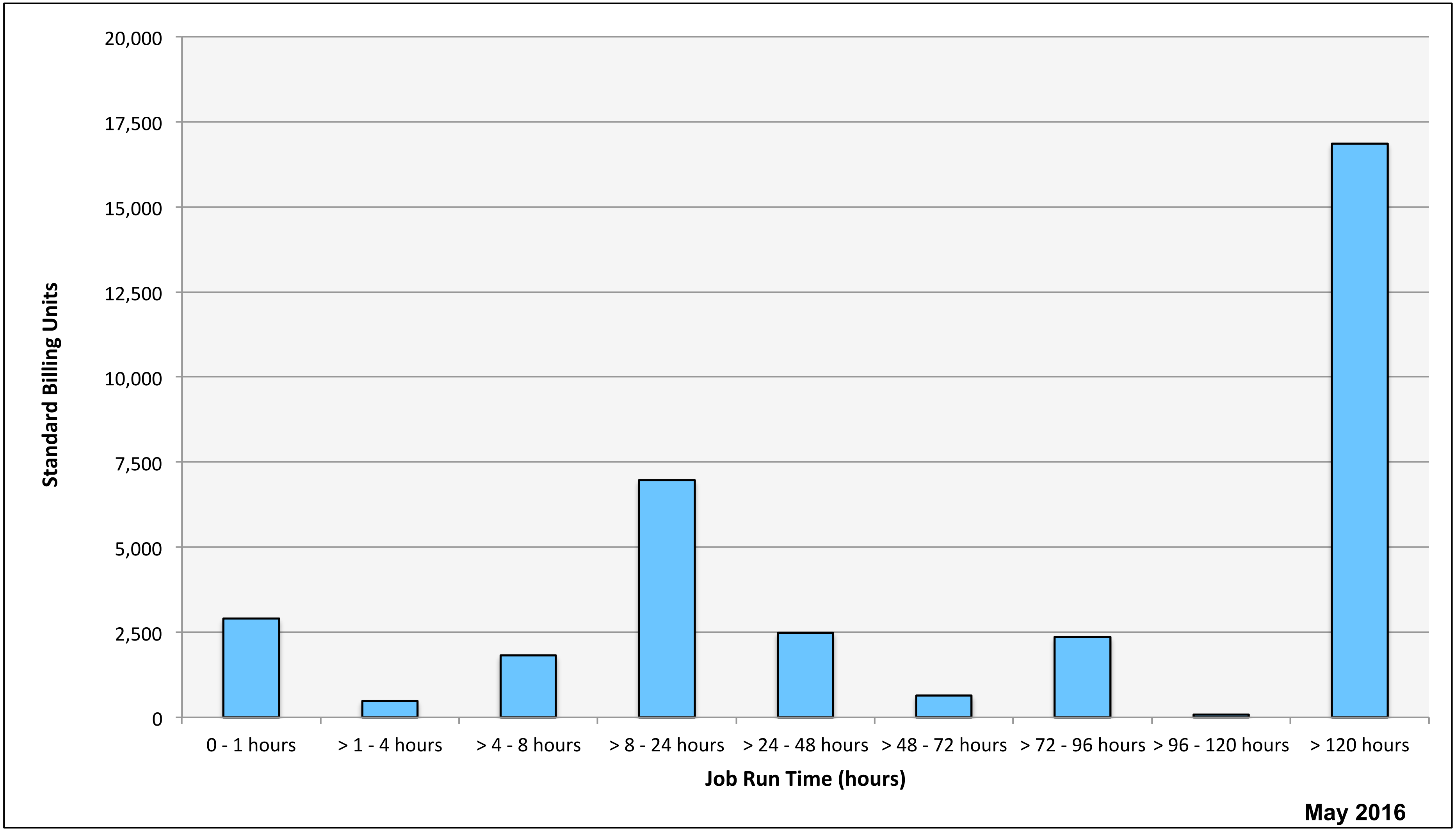
Pleiades: Average Expansion Factor



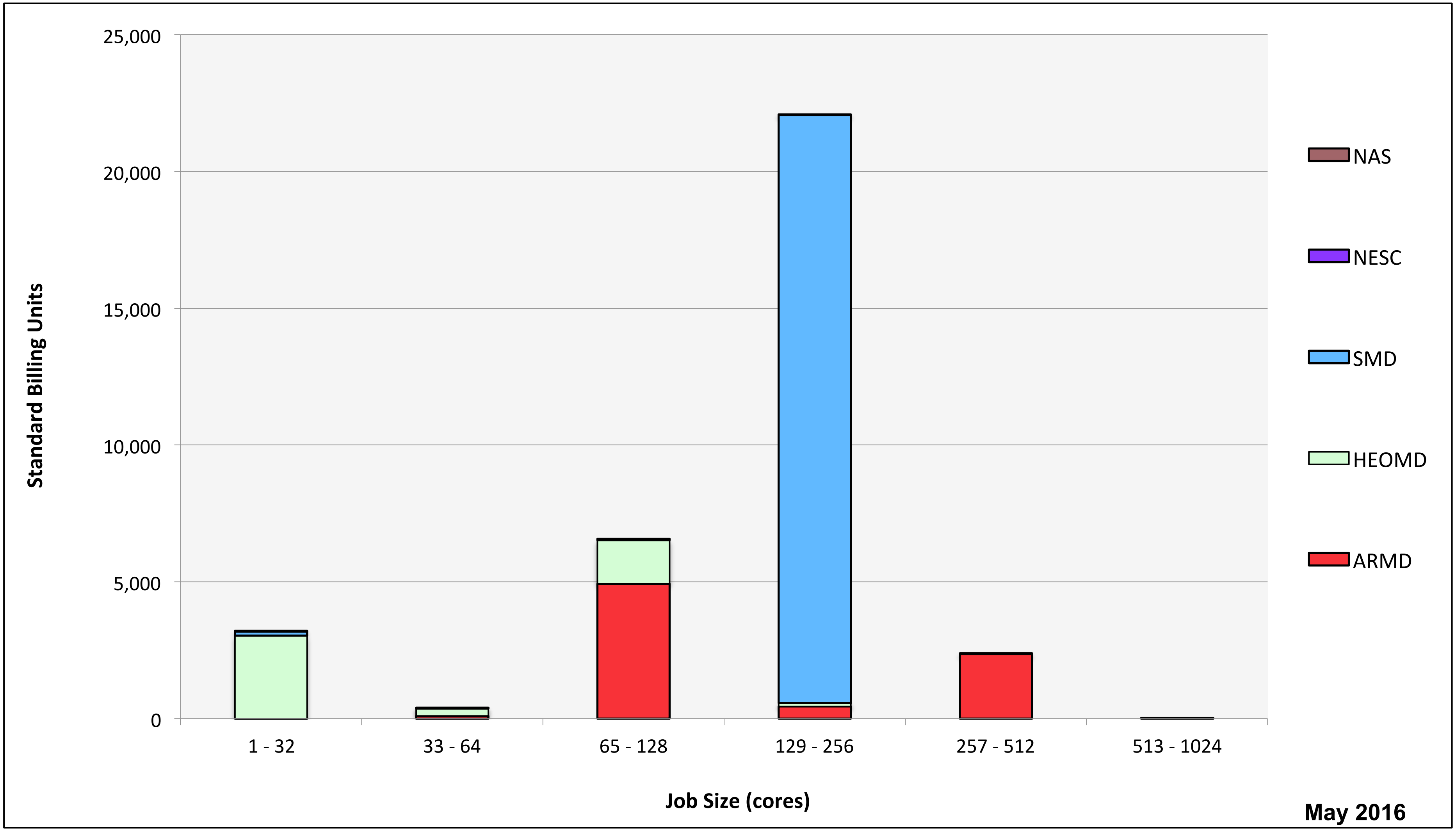
Endeavour: SBUs Reported, Normalized to 30-Day Month



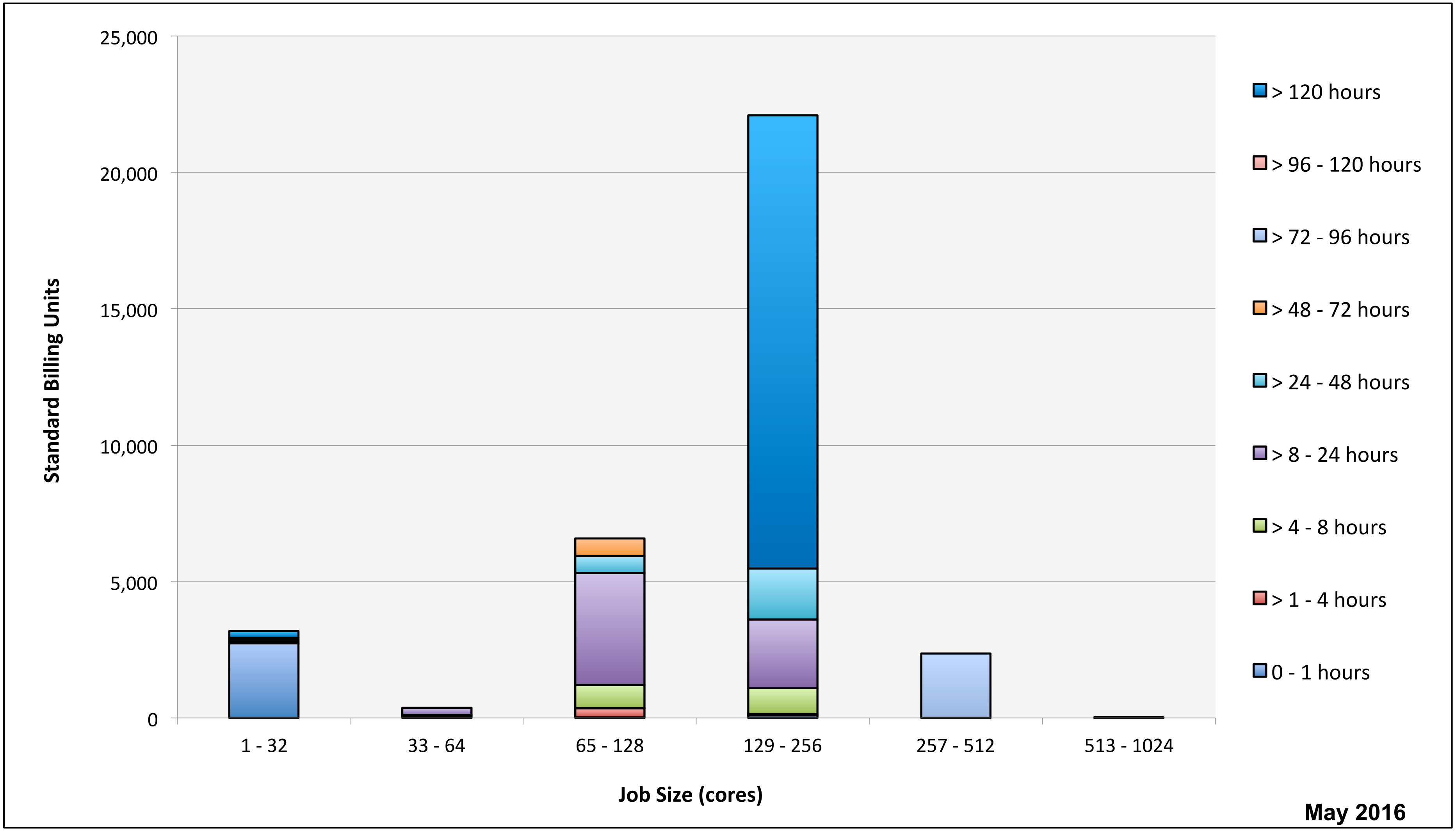
Endeavour:
Monthly Utilization by Job Length



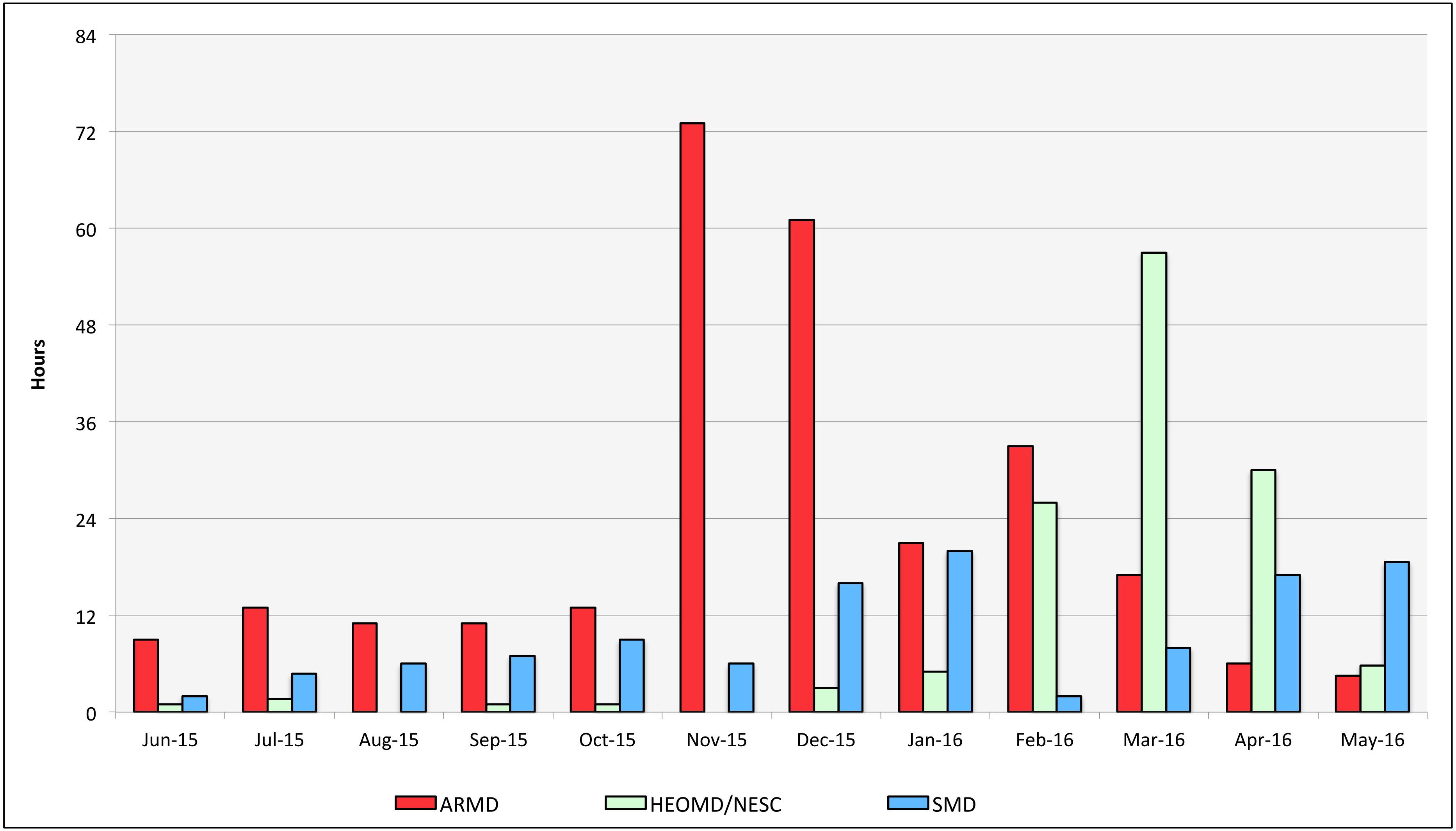
Endeavour:
Monthly Utilization by Size and Mission



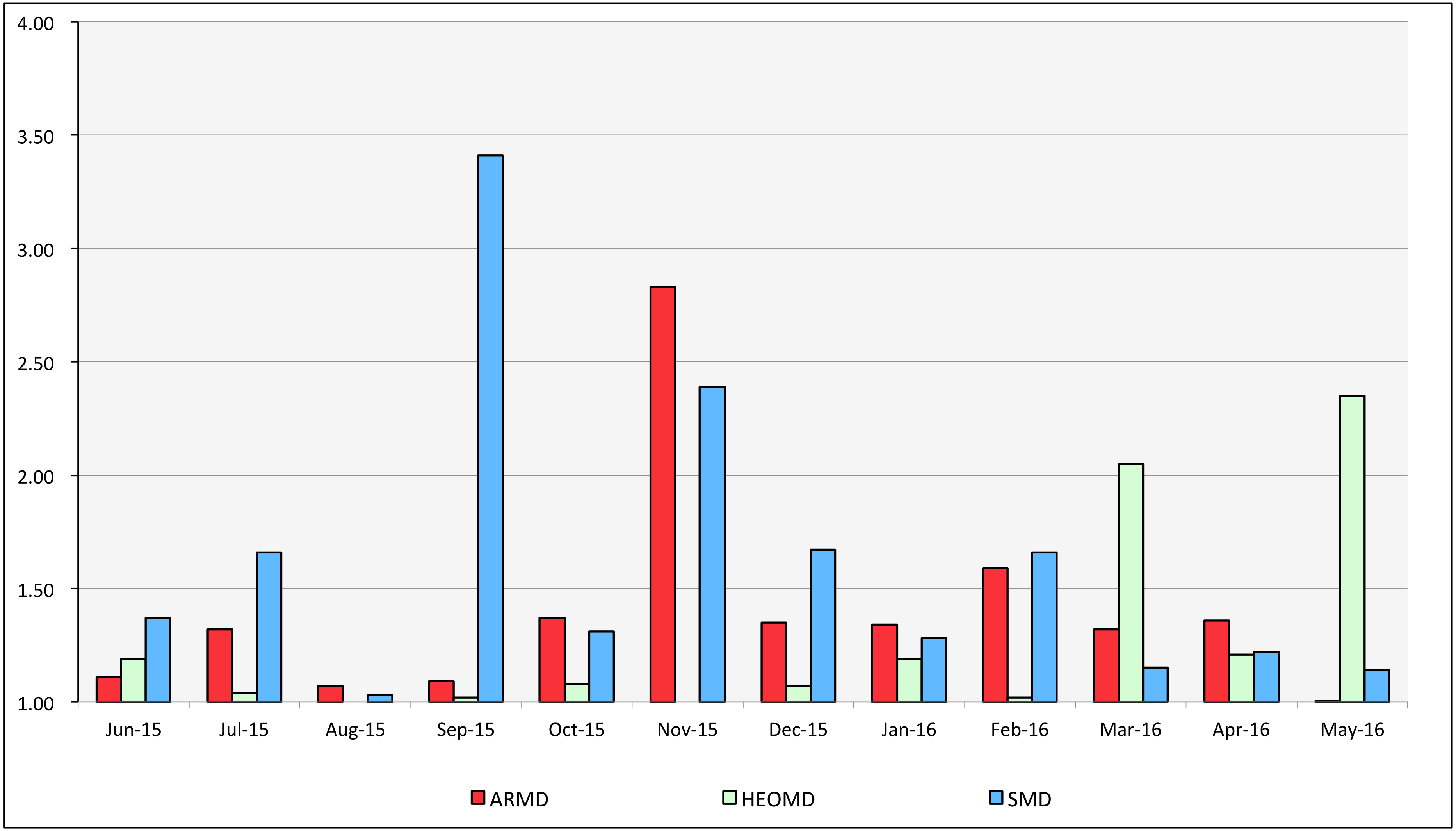
Endeavour:
Monthly Utilization by Size and Length



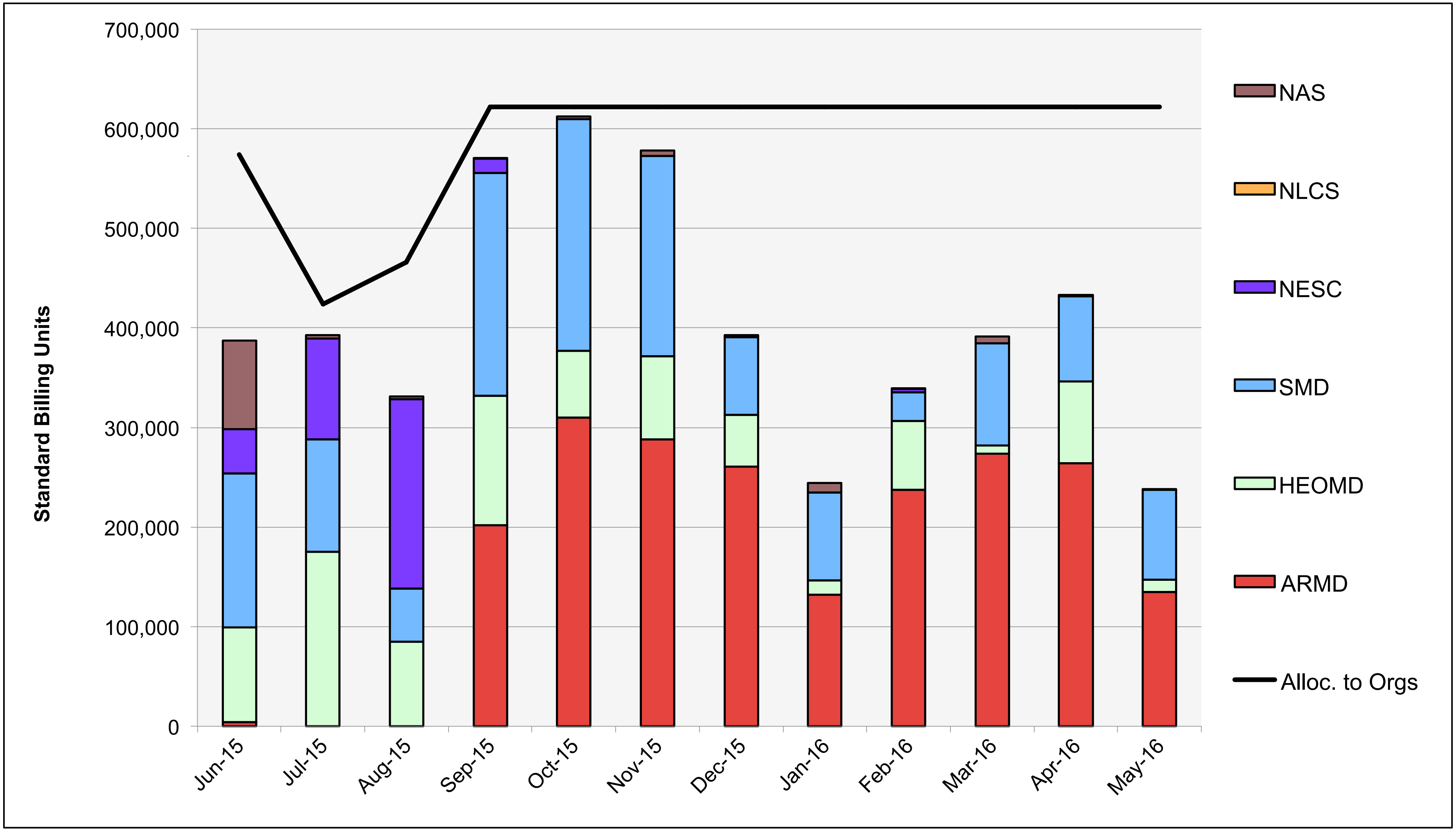
Endeavour: Average Time to Clear All Jobs



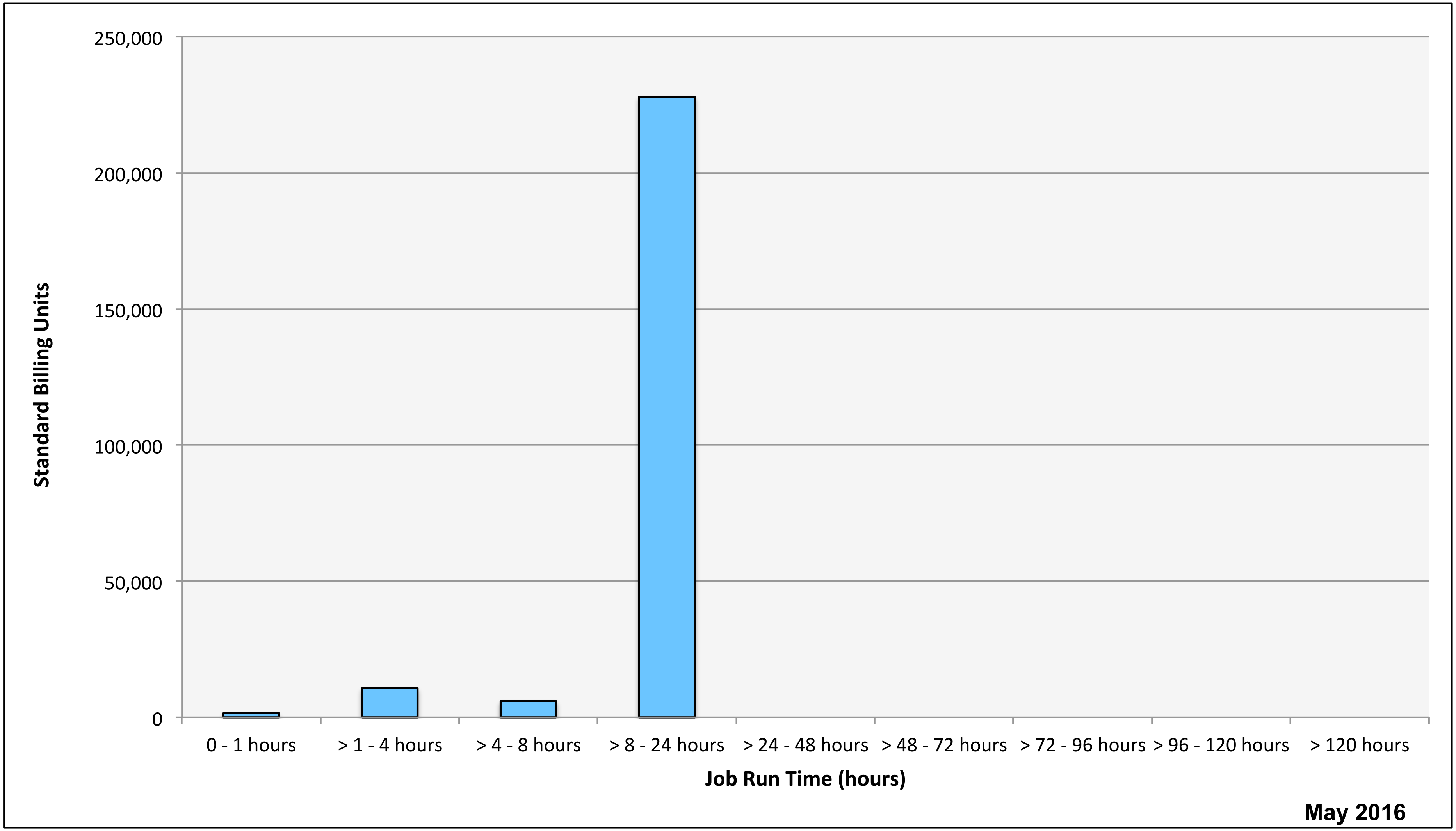
Endeavour: Average Expansion Factor



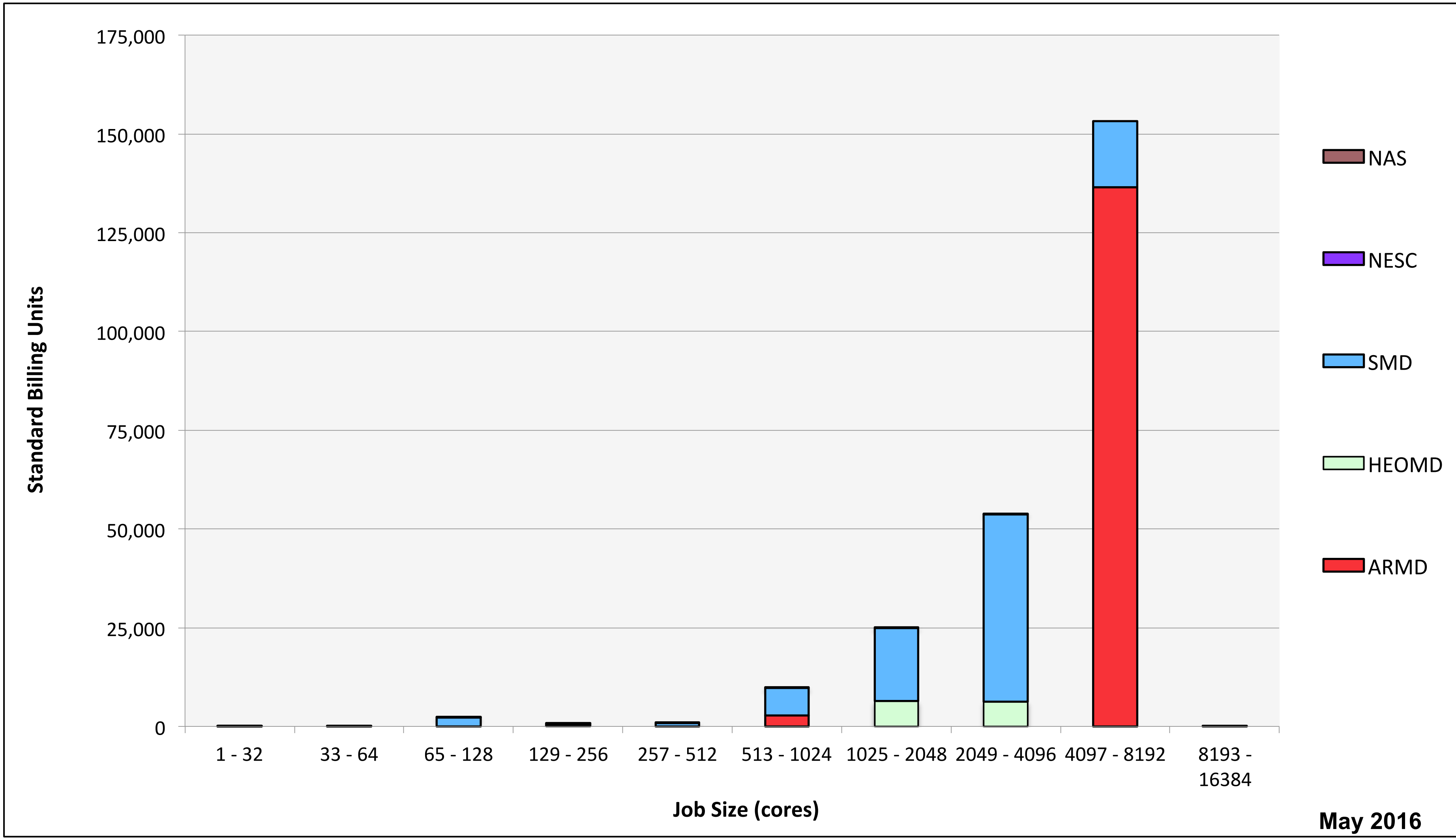
Merope:
SBUs Reported, Normalized to 30-Day Month



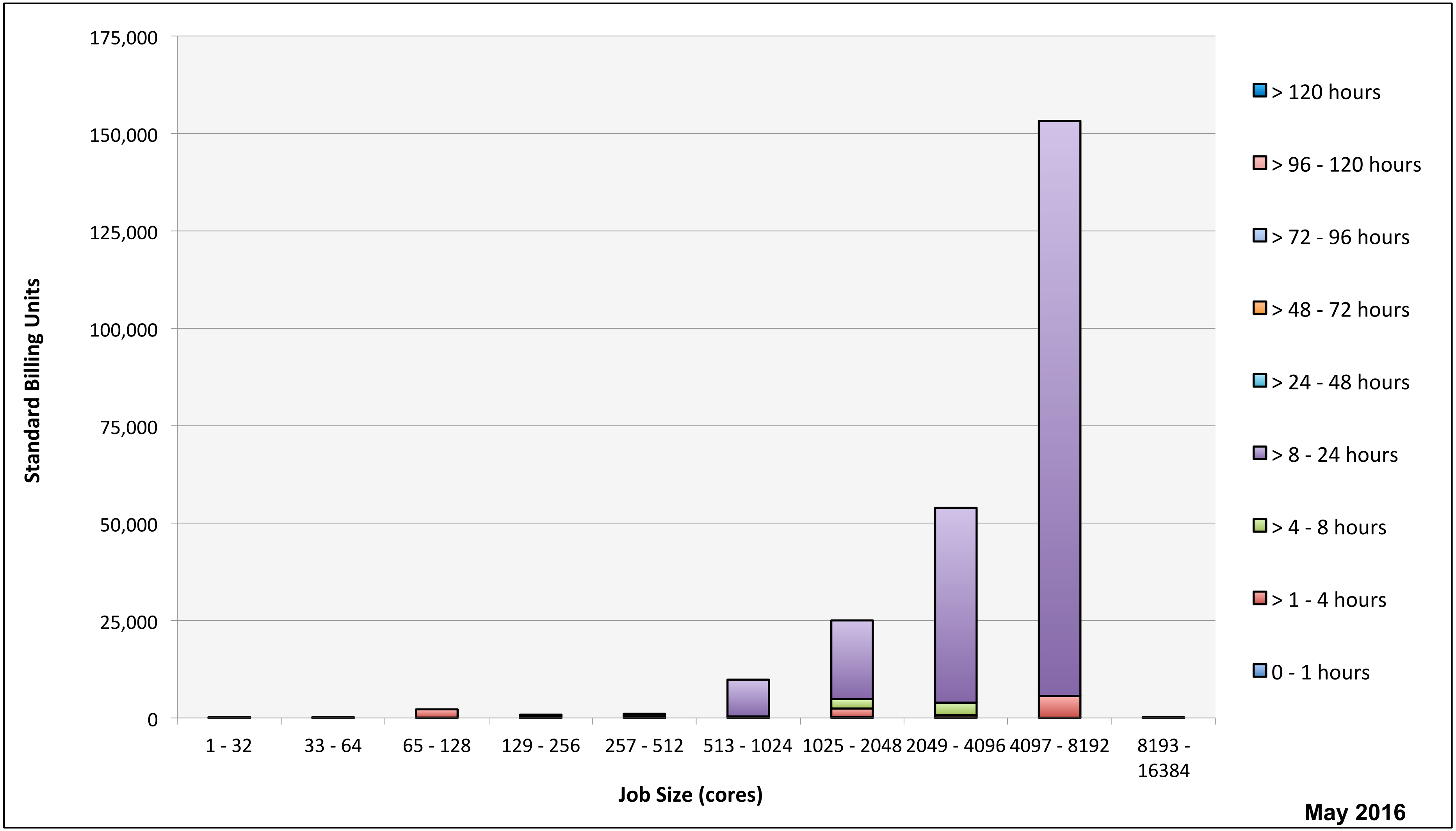
Merope: Monthly Utilization by Job Length



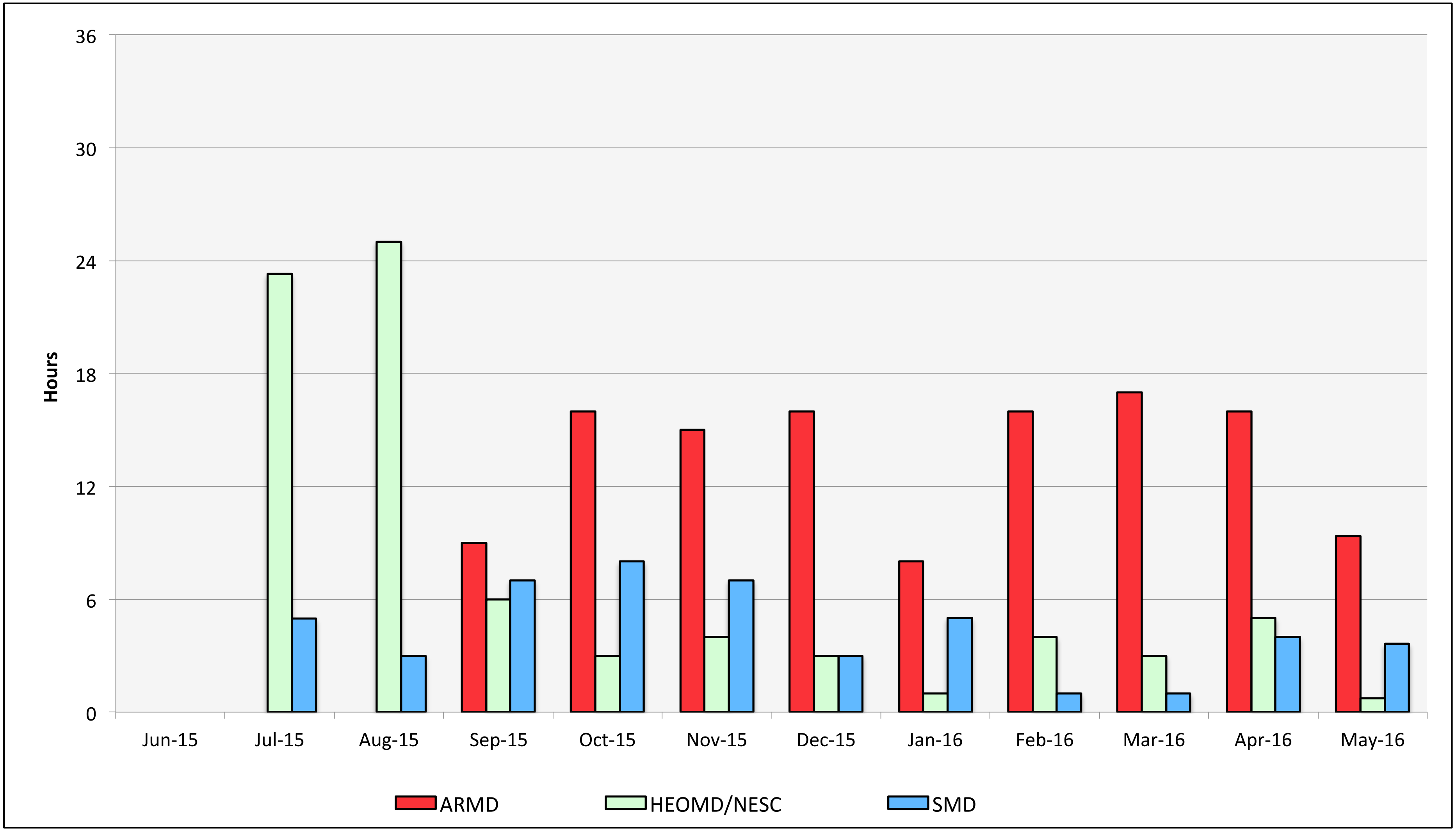
Merope:
Monthly Utilization by Size and Mission



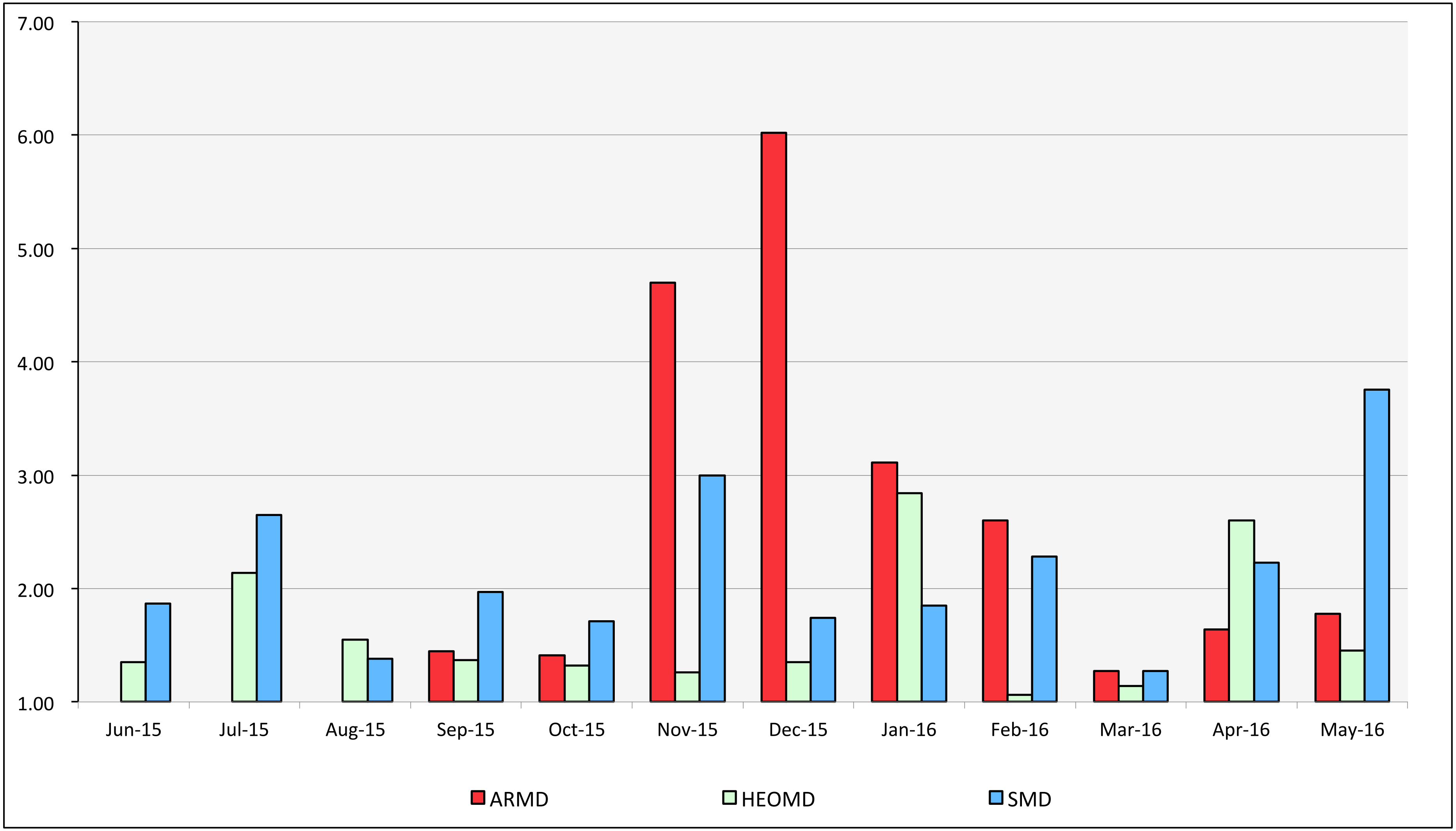
Merope:
Monthly Utilization by Size and Length

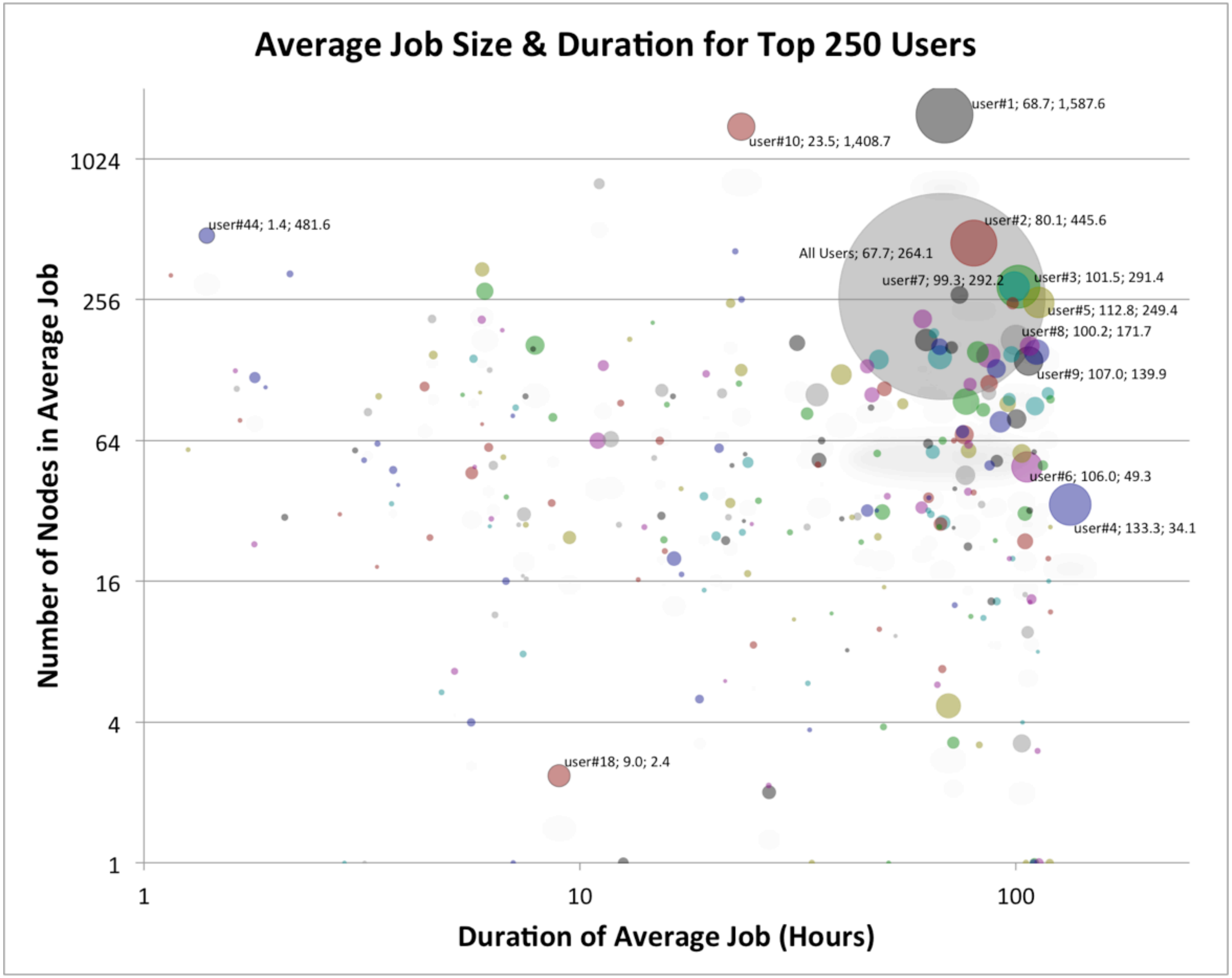


Merope: Average Time to Clear All Jobs



Merope:
Average Expansion Factor




Average Job Size & Duration for Top 250 Users
Number of Nodes in Average Job
Duration of Average Job (Hours)
1024
256
64
16
4
1
1
10
100
user#1; 68.7; 1,587.6
user#10; 23.5; 1,408.7
user#44; 1.4; 481.6
user#2; 80.1; 445.6
All Users; 67.7; 264.1
user#7; 99.3; 292.2
user#3; 101.5; 291.4
user#5; 112.8; 249.4
user#8; 100.2; 171.7
user#9; 107.0; 139.9
user#6; 106.0; 49.3
user#4; 133.3; 34.1
user#18; 9.0; 2.4