Project Status Report

High End Computing Capability
Strategic Capabilities Assets Program

November 10, 2017

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Electra Skylake Expansion Released For Production

- HECC released the new Skylake expansion of the Electra supercomputer for general availability after extensive testing by users and HECC staff.
- The expansion adds 1,152 Skylake nodes to the existing Broadwell Electra nodes. The system's total peak performance is now 4.78 petaflops.
- A standard billing unit (SBU*) rate of 6.36 was calculated for the Skylake nodes—1.58 times the rate for a Broadwell node.
- The Skylake nodes are configured to automatically mount the required filesystems to run users' applications, in order to reduce the amount of memory used. This results in more memory available for user applications on the compute nodes. This functionality will be deployed to all other HECC systems in the near future.

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

The first Electra module with Broadwell processors was augmented with a second module containing the latest generation of Intel Xeon Gold 6148 Skylake processors.

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

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

HECC Improves Tape Library Performance

- HECC improved the tape drive performance in the archive system by tuning parameters to enable more efficient usage.
- The LTO7 tape drives are capable of 300 megabytes/second (MB/s) of native performance, but were experiencing significantly slower performance—as low as 30 MB/s for large files. This can adversely impact the lifespan of the media, as well as the amount of data stored on tape.
- Making a configuration change to avoid direct I/O reads from disk/writes to tape increased tape writes to achieve near-line-rate performance while improving the tape throughput.
- These updates will significantly improve the migration speed of more than 60 petabytes of data from the LTO5 to the current LTO7 generation of drives.

Mission Impact: Enhancing the performance of archive systems is critical to keeping pace with the ever-increasing data storage requirements of science and engineering users supporting agency missions.

The HECC archive system has over 178 petabytes of dual-copy data that is stored across six tape libraries.

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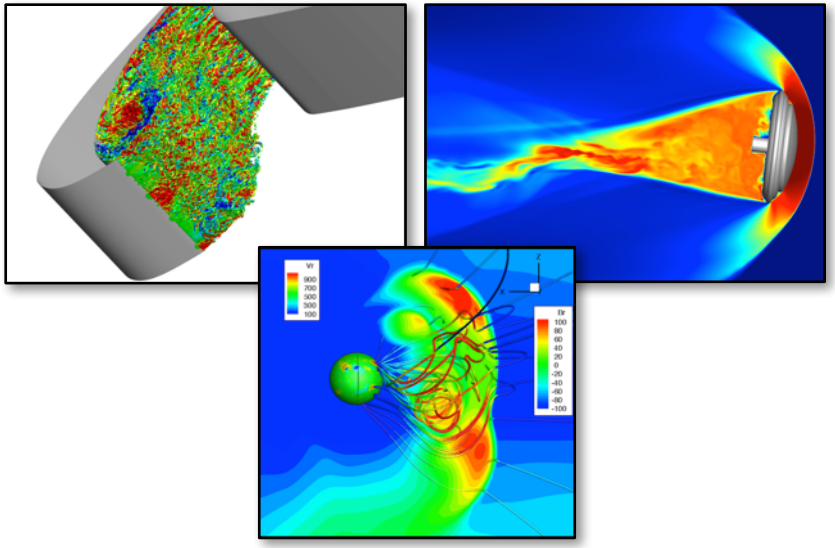
New Allocation Period for Supercomputer Time Begins for NASA Mission Directorates

- October 1 was the start of the new allocation period for all of NASA's mission directorates.
- The mission directorates awarded about 306 million SBUs* of supercomputer time on HECC systems to 455 projects.
- The Aeronautics Research Mission Directorate (ARMD) awarded over 92 million SBUs to 138 projects.
- The Human Exploration and Operations Mission Directorate (HEOMD) awarded about 91 million SBUs to 64 projects.
- The Science Mission Directorate (SMD) awarded almost 123 million SBUs to 253 projects.
- Installation of Electra in Jan. 2017, allowed ARMD to award 15% more SBUs than last year, while HEOMD awarded 21% more.
- SMD is phasing their awards over the coming year, and so initially awarded only about 72% of its share.

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.



Images representing the variety of projects supported by HECC resources. Clockwise from top left: 1) Isocontour of streamwise vorticity that highlights the wake generated from the leading edge of an aircraft slat. *Jeff Housman, NASA/Ames*; 2) Visualization of the temperature around a free-flying model tested in the NASA Ames Ballistic Range. *Joe Brock, NASA/Ames*; 3) Coronal mass ejection propagation simulation. *Antonia Savcheva, NASA/Ames & Harvard-Smithsonian Center for Astrophysics.*

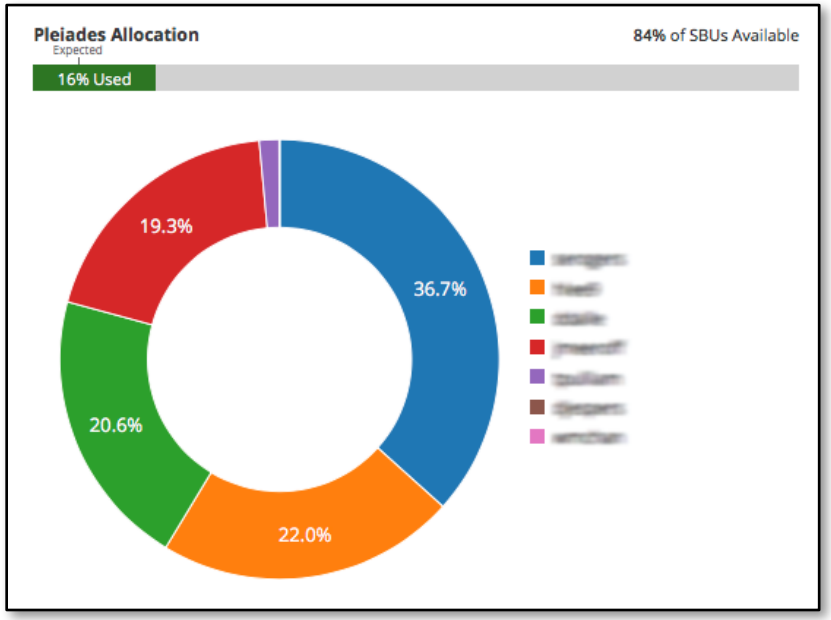
POC: Catherine Schulbach, catherine.h.schulbach@nasa.gov, (650) 604-3180, NASA Advanced Supercomputing Division.

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

myNAS Website Released to Principal Investigators (PIs)

- The HECC Tools team released the PI edition of the myNAS website to HECC principal investigators. This site provides PIs with near-real-time information on running, waiting, held, and recently finished jobs across all their GIDs. Job listings can be filtered by users, machines, queues, models, and other parameters. PIs can also view utilization bar and donut charts, which show detailed allocation and accounting information at a glance.
- The Tools team collaborated with the Application Performance & Productivity team to develop the myNAS website, which is hosted on the new portal.nas.nasa.gov server. PIs must authenticate using Launchpad, with either a NASA Smartcard or RSA token, to access the site.
- myNAS uses 18 scripts and 5 API calls to gather, store, process, and present detailed information on thousands of active and completed jobs, updated for PIs every about every 10 minutes.
- After incorporating feedback on site features from PI beta testers, the Tools team performed code optimizations that sped up back-end database operations ~72% and browser page loading ~400%.
- The Tools team is planning a release of the myNAS website for individual users in the near future.

Mission Impact: The myNAS website provides principal investigators with new tools to analyze and optimize their use of HECC resources.



The myNAS accounts page shows PIs key usage data for each of their GIDs at a glance. This screenshot features a bar graph with the percentage of total GID allocation used to date vs. expected (linear) usage. The donut chart indicates the relative amount used by each GID member.

POCs: John Hardman, john.hardman@nasa.gov, (650) 604-0417, NASA Advanced (NAS) Supercomputing Division, CSRA LLC; Ryan Spaulding, ryan.c.spaulding@nasa.gov, (408) 772-6567, NAS Division, ADNET Systems

HECC Supercomputer Usage in October 2017 Tops 28 Million SBUs

- In October, the combined usage on HECC supercomputers (including free testing time) set a new record of 28,142,305 Standard Billing Units (SBUs*).
- The usage by 359 of NASA's science and engineering groups exceeded May's record of 25,690,988 SBUs by more than 2.4 million SBUs, or by about 9.5%.
- Usage of Pleiades, Electra, Merope, and Endeavour contributed to this record.
- The record was primarily enabled by the addition of 1,152 Skylake nodes to Electra—an increase that nearly quadrupled the system's peak performance.
- The top 10 projects used between 508,526 and 2,049,280 SBUs, and together accounted for over 38% of the total usage.
- The HECC Project continues to plan and evaluate ways to address the future requirements of NASA's users.

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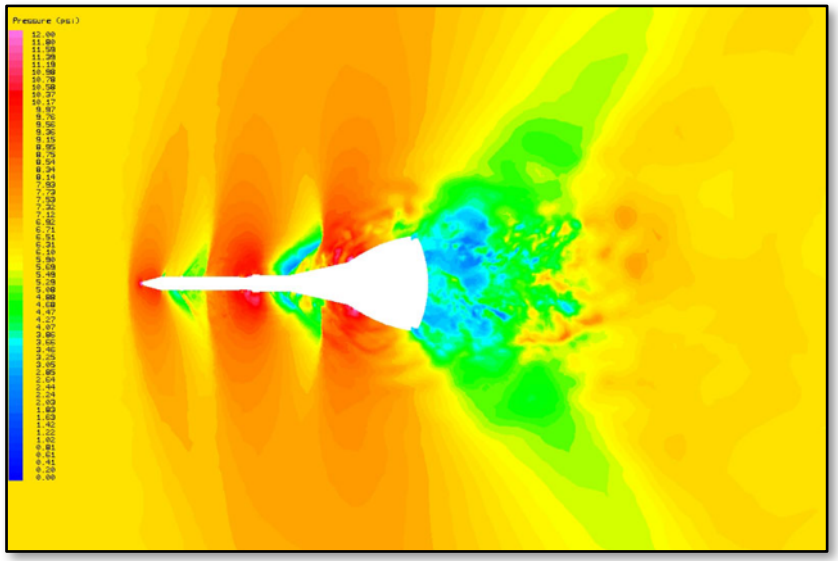
Mission Impact: Increasing the capacity of HECC systems provides mission directorates with more resources to accomplish their goals and objectives.



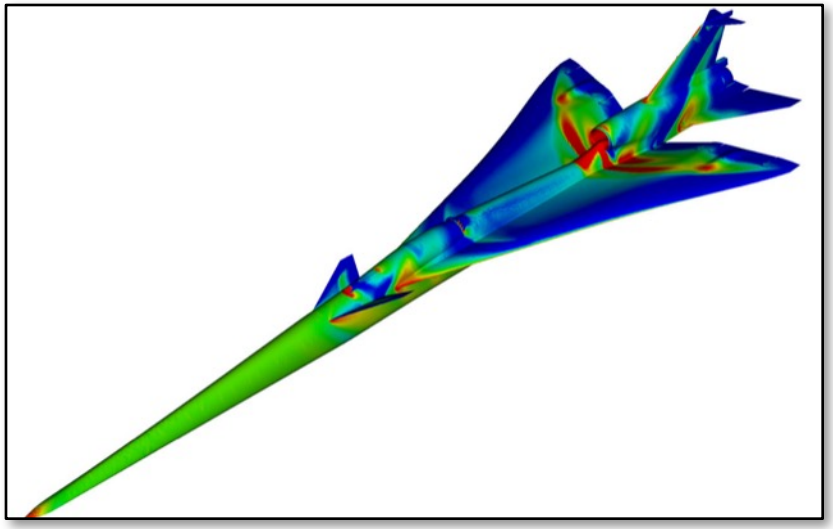
Example of work done on HECC systems. This snapshot shows pressure contours and the complex, unsteady flow features around the Orion Launch Abort Vehicle and, particularly, around the crew capsule. *Josh Rojahn, NASA/MSFC*

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

Pleiades Simulations Support the Design of Quiet Supersonic Aircraft

- Researchers are running simulations on Pleiades to examine the noise level that would be produced by the Low Boom Flight Demonstrator (LBFD), an experimental X-plane currently being developed by NASA engineers.
- Run using NASA's Launch Ascent and Vehicle Aerodynamics (LAVA) solver, the computational fluid dynamics simulations provide accurate modeling of both the aircraft and the flow field that occurs in its vicinity.
  - The researchers generate a computational model of the full aircraft and its nearby airspace, which requires 50 to 100 million grid cells for each design.
  - The pressure signatures of each LBFD design are extracted from the simulations and used to determine the sonic boom loudness level.
- Results from these simulations help the LBFD designers assess the sonic boom performance of each new design.
- The X-plane built from the final LBFD design will be used to conduct flight tests to evaluate the validity of a quiet supersonic design.

Mission Impact: Simulations run on HECC resources help NASA engineers ensure that the Low Boom Flight Demonstrator design can meet extremely stringent sonic boom loudness levels, supporting the agency's goal of achieving practical supersonic passenger jet travel over land.



Visualization of the pressure field over the Low Boom Flight Demonstrator (LBFD). This type of visualization can help diagnose what parts of the aircraft correspond to certain features in the extracted shock signatures. *James Jensen, NASA/Ames*

POCs: James Jensen, james.c.jensen@nasa.gov, (650) 604-2640, Cetin Kiris, cetin.c.kiris@nasa.gov, (650) 604-4485; NASA Advanced Supercomputing Division

HECC Facility Hosts Several Visitors and Tours in October 2017

- HECC hosted 10 tour groups in October; 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:
  - Chris Stewart, Congressman from Utah's second district and Republican Chair, Subcommittee on Department of Defense Intelligence Overhead Architecture; and five congressional staff members; along with high-level management from Hewlett Packard Enterprise, were given a HECC briefing. The committee attended a meeting at Stanford University's Hoover Institution regarding the importance of HPC to the Intelligence community.
  - Jen Rae Wang, NASA Associate Administrator, Office of Communications, received a HECC/NAS overview and hyperwall demonstration, and toured the main supercomputer room and quantum computer room.
  - Researchers and professors from the Norwegian University of Science & Technology, who visited for technical discussions with the Ames Small Satellite Division.
  - Japanese visitors from Obayashi Corporation, known for their proposal to construct a space elevator by 2050. NASA is working with them on ideas for building habitats in space.
  - A delegation from the United Negro College Fund and Historically Black Colleges and Universities toured Ames to collaborate on future educational opportunities for students.
  - A group of students from a Computational Physics class from California State University, East Bay visited Ames and received a HECC and quantum computing overview and tour.
  - The actor Sean Penn requested and received a tour of Ames, including the NAS facility, while visiting the independent company Vasper Systems at NASA Research Park.

Congressman Chris Stewart (4th from left) and congressional staff members received an HECC overview and tour during their visit to Ames.

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

Papers

- "**Gravity Wave Variation from the Troposphere to the Lower Thermosphere during a Stratospheric Sudden Warming Event: A Case Study**," H.-L. Liu, SOLA, vol. 13A, Special Edition, October 2, 2017. *
  https://www.jstage.jst.go.jp/article/sola/13A/Special_Edition/13A_13A-005/_article
- "**The Effect of Turbulence on Nebular Emission Line Ratios**," W. Gray, E. Scannapieco, arXiv:1710.01312 [astro-ph.GA], October 3, 2017. *
  https://arxiv.org/abs/1710.01312
- "**Sequence-Dependent Interfacial Adsorption and Permeation of Dipeptides Across Phospholipid Membranes**," C. Wei, A. Pohorille, The Journal of Physical Chemistry B, October 5, 2017. *
  http://pubs.acs.org/doi/abs/10.1021/acs.jpcb.7b08238
- "**3D Kinetic Pulsar Magnetosphere Models: Exploring Self Consistency**," C. Kalapotharakos, et al., arXiv:1710.03170 [astro-ph.HE], October 9, 2017. *
  https://arxiv.org/abs/1710.03170
- "**Simulation of Mesoscale Cellular Convection in Marine Stratocumulus. Part I: Drizzling Conditions**," X. Zhou, et al., Journal of the Atmospheric Sciences, vol. 74, no. 11, published online October 11, 2017. *
  http://journals.ametsoc.org/doi/abs/10.1175/JAS-D-17-0070.1
- "**Instability Wave-Streak Interactions in a Supersonic Boundary Layer**," P. Paredes, M. Choudhari, F. Li, Journal of Fluid Mechanics, vol. 831, published online October 13, 2017. *
  https://doi.org/10.1017/jfm.2017.630

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

Papers (cont.)

- "**Large-Eddy Simulation of Flow Over a Wall-Mounted Hump with Separation and Reattachment**," A. Uzun, M. Malik, AIAA Journal, published online October 16, 2017. * https://arc.aiaa.org/doi/abs/10.2514/1.J056397
- "**On the Deceleration and Spreading of Relativistic Jets I: Jet Dynamics**," P. Duffell, T. Laskar, arXiv:1710.07253 [astro-ph.HE], October 19, 2017. * https://arxiv.org/abs/1710.07253
- "**Kinetic Simulation Technique for Plasma Flow in Strong External Magnetic Field**," F. Ebersohn, J. Sheehan, A. Gallimore, J. Shebalin., Journal of Computational Physics, vol. 351, published online October 19, 2017. * http://www.sciencedirect.com/science/article/pii/S0021999117306800
- "**Collapsed Carbon Nanotubes as Building Blocks for High-Performance Thermal Materials**," J. Al-Ghalith, H. Xu, T. Dumitrică, Physical Review Materials, October 25, 2017. * https://journals.aps.org/prmaterials/abstract/10.1103/PhysRevMaterials.1.056001
- "**Radiative Cooling of Swept Up Gas in AGN-Driven Galactic Winds and Its Implications for Molecular Outflows**," A. Richings, C.-A. Faucher-Giguere, arXiv:1710.09433 [astro-ph.GA], October 25, 2017. * https://arxiv.org/abs/1710.09433
- "**Does the Galaxy-Halo Connection Vary with Environment?**," R. Dragomir, A. Rodriguez-Puebla, J. Primack, C. Lee., arXiv:1710.09392 [astro-ph.GA], October 25, 2017. * https://arxiv.org/abs/1710.09392

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Presentations

- "**Interactive Visualization of High-Dimensional Petascale Ocean Data**," D. Ellsworth, C. Henze, B. Nelson, presented at the 7th IEEE Symposium on Large Data Analysis and Visualization, Phoenix, AZ, October 2, 2017.
- "**Recent Developments in Accuracy and Stability Improvement of Nonlinear Filter Methods for DNS and LES of Compressible Flows**," H. Yee, keynote speech presented at the 2nd International Conference on Fluid Dynamics and Aerodynamics, Rome, Italy, October 19-20, 2017.* *http://fluid-aerodynamics.global-summit.com/abstract/2017/recent-developments-in-accuracy-and-stability-improvement-of-nonlinear-filter-methods-for-dns-and-les-of-compressible-flows*

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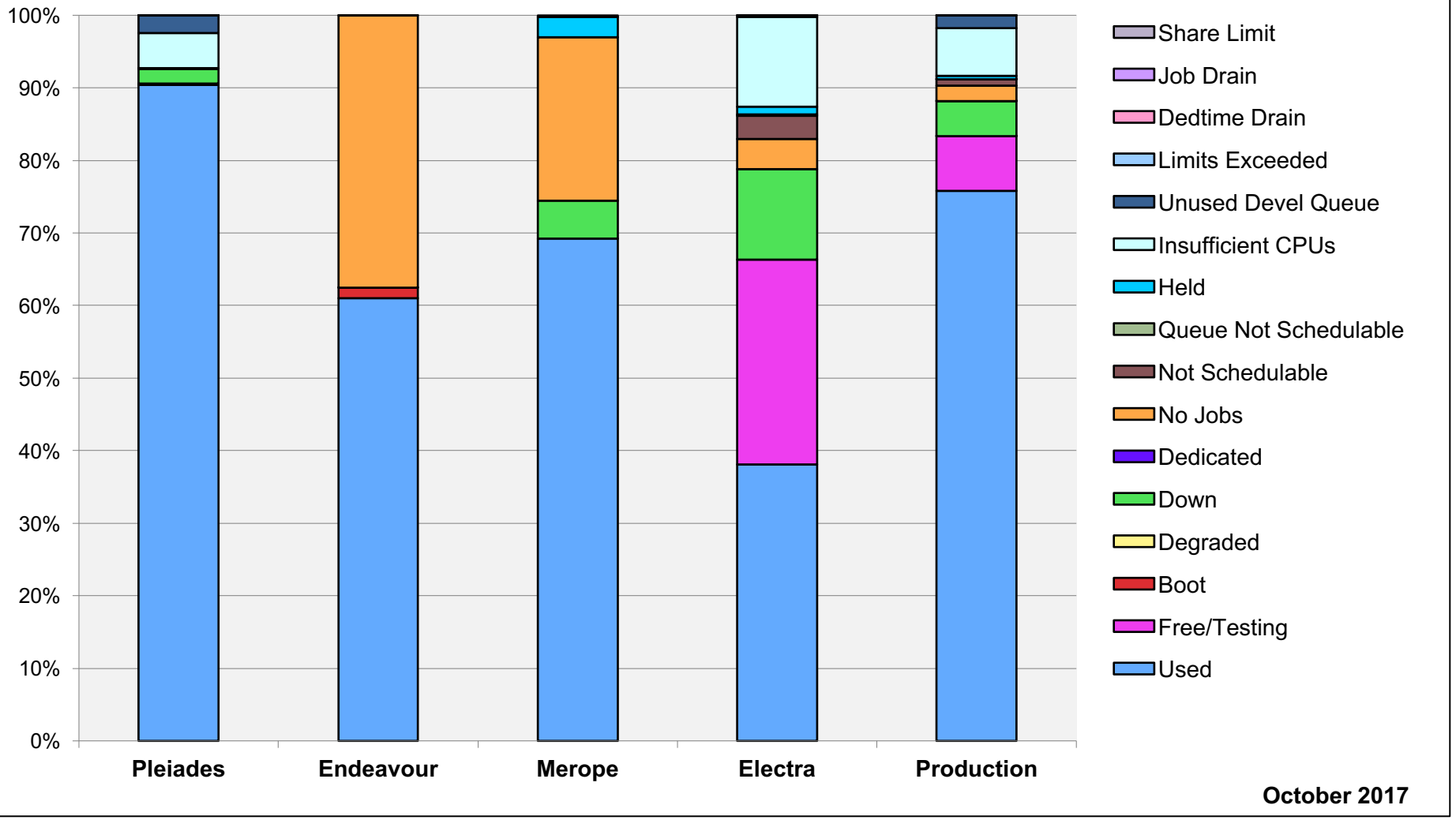
News and Events

- **NASA Researcher Wins CFD Flow Visualization Award**, K. Pitta, NAS News, October 10, 2017—Patrick Blonigan, a USRA researcher at the NASA Advanced Supercomputing Division, received the award for Most Quantitatively Descriptive Flow Visualization Animation at the CFD Flow Visualization Showcase held during the 2017 AIAA Aviation Forum and Exhibition in Denver, CO.
  https://www.nas.nasa.gov/publications/news/2017/10-17-17.html
- **Video: NASA Advanced Computing Environment for Science & Engineering**, *insideHPC*, October 15, 2017—NASA's Rupak Biswas presents his talk "NASA Advanced Computing Environment for Science & Engineering" from the 2017 Argonne Training Program on Extreme-Scale Computing.
  https://insidehpc.com/2017/10/video-nasa-advanced-computing-environment-science-engineering/
- **SC17 Video Dives into How Supercomputers and Scientific Visualization are Helping Us Understand the Ocean's Role in Weather and Climate**, J. Dunbar, SC17 Blog Post, October 19, 2017–A video just released by SC17 conference relates how scientists are zooming in on one of the highest-resolution computer simulations in the world to explore never-before-seen features of the global ocean eddies and circulation.
  http://sc17.supercomputing.org/2017/10/19/video-dives-into-how-supercomputers-and-scientific-visualization-are-helping-us-understand-the-oceans-role-in-weather-and-climate/
  - **#HPCConnects – Ocean Mapping**, *SC Conferences YouTube*, October 19, 2017.
    https://www.youtube.com/watch?v=aLdNDFuLazw

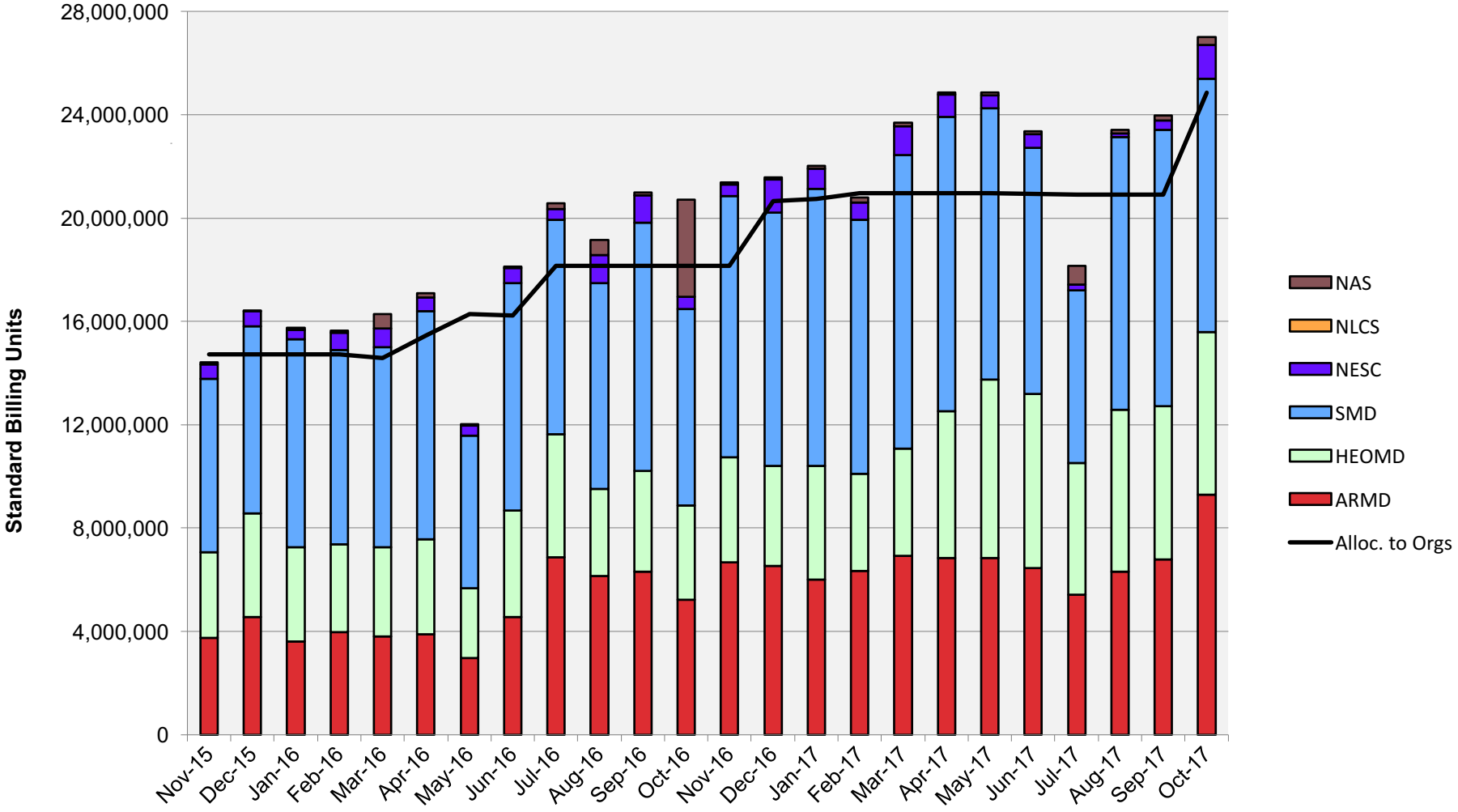
News and Events

- **Adam Moreno Talks About Supercomputing for Global Systems**, *NASA in Silicon Valley Podcast*, October 19, 2017—NASA's Matthew Buffington talks to Adam Moreno, scientist with the NASA Earth Exchange program, which works to bring global research datasets and make them public so that any researcher in the world can make use of the information.
  https://www.nasa.gov/ames/nisv-podcast-Adam-Moreno
- **Bron Nelson and Dimitris Menemenlis Talk About Modeling Oceans and Ice with Supercomputers**, *NASA in Silicon Valley Podcast*, October 26, 2017—Matthew Buffington talks with Bron Nelson (NASA Advanced Supercomputing Division) and Dimitris Menemenlis (NASA's Jet Propulsion Laboratory) about how they are utilizing supercomputing resources and new interactive visualization tools like the NAS hyperwall to explore high-resolution models of Earth's oceans.
  https://www.nasa.gov/ames/nisv-podcast-Bron-Nelson-Dimitris-Menemenlis

HECC Utilization



HECC Utilization Normalized to 30-Day Month



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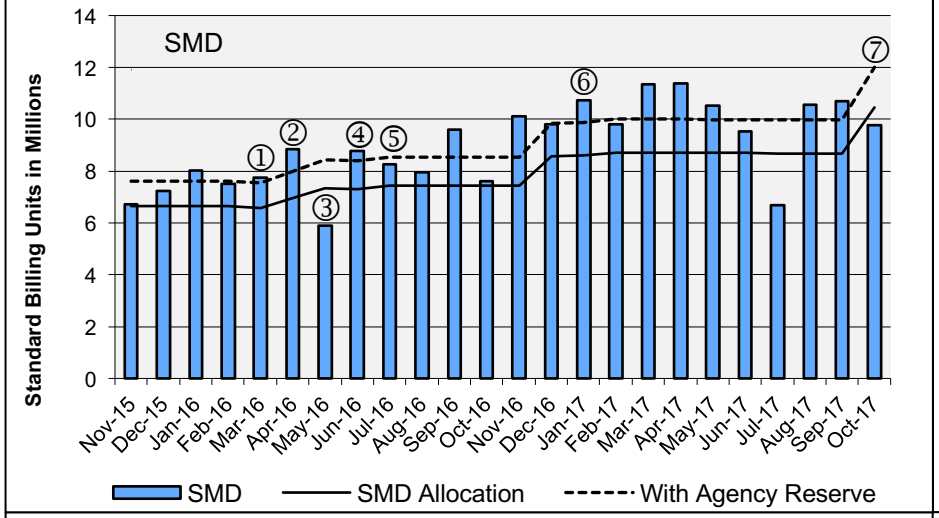
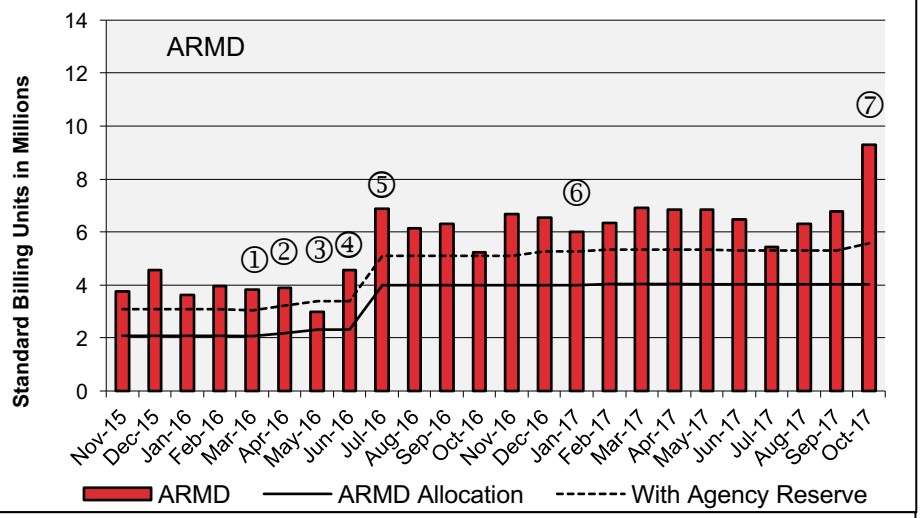
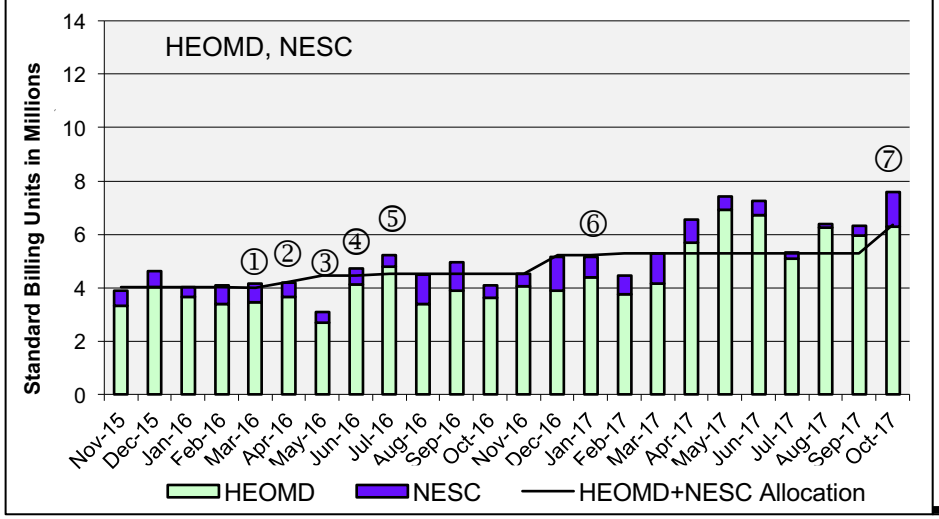
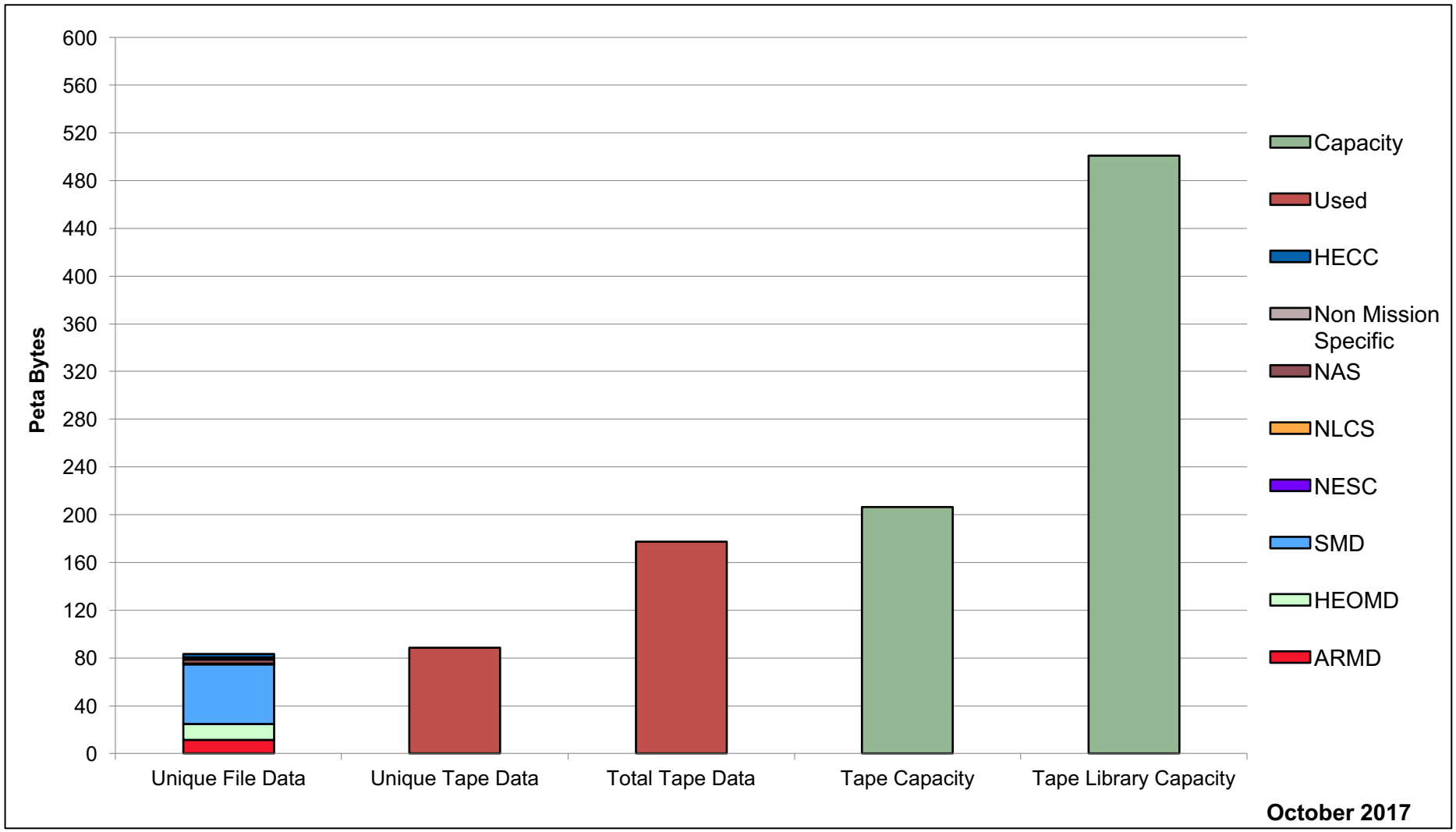






① 16 Westmere racks retired from Pleiades
② 10 Broadwell racks added to Pleiades
③ 4 Broadwell racks added to Pleiades
④ 14 (All) Westmere racks retired from Pleiades
⑤ 14 Broadwell Racks added to Pleiades
⑥ 16 Electra Broadwell Racks in Production, 20 Westmere 1/2 racks added to Merope
⑦ 4 Skylake E Cells (16 D rack equivalents) added to Electra

Tape Archive Status



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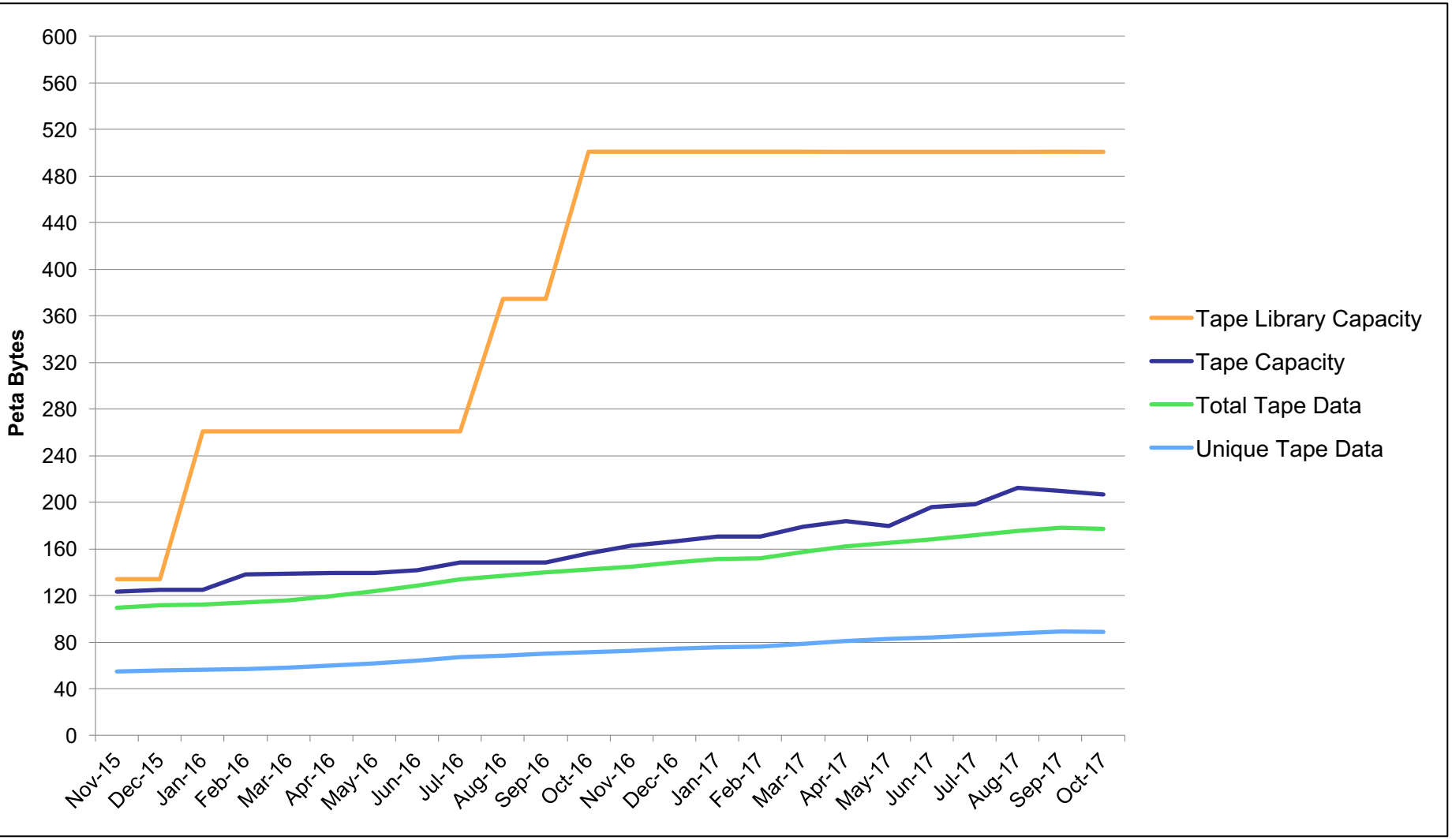
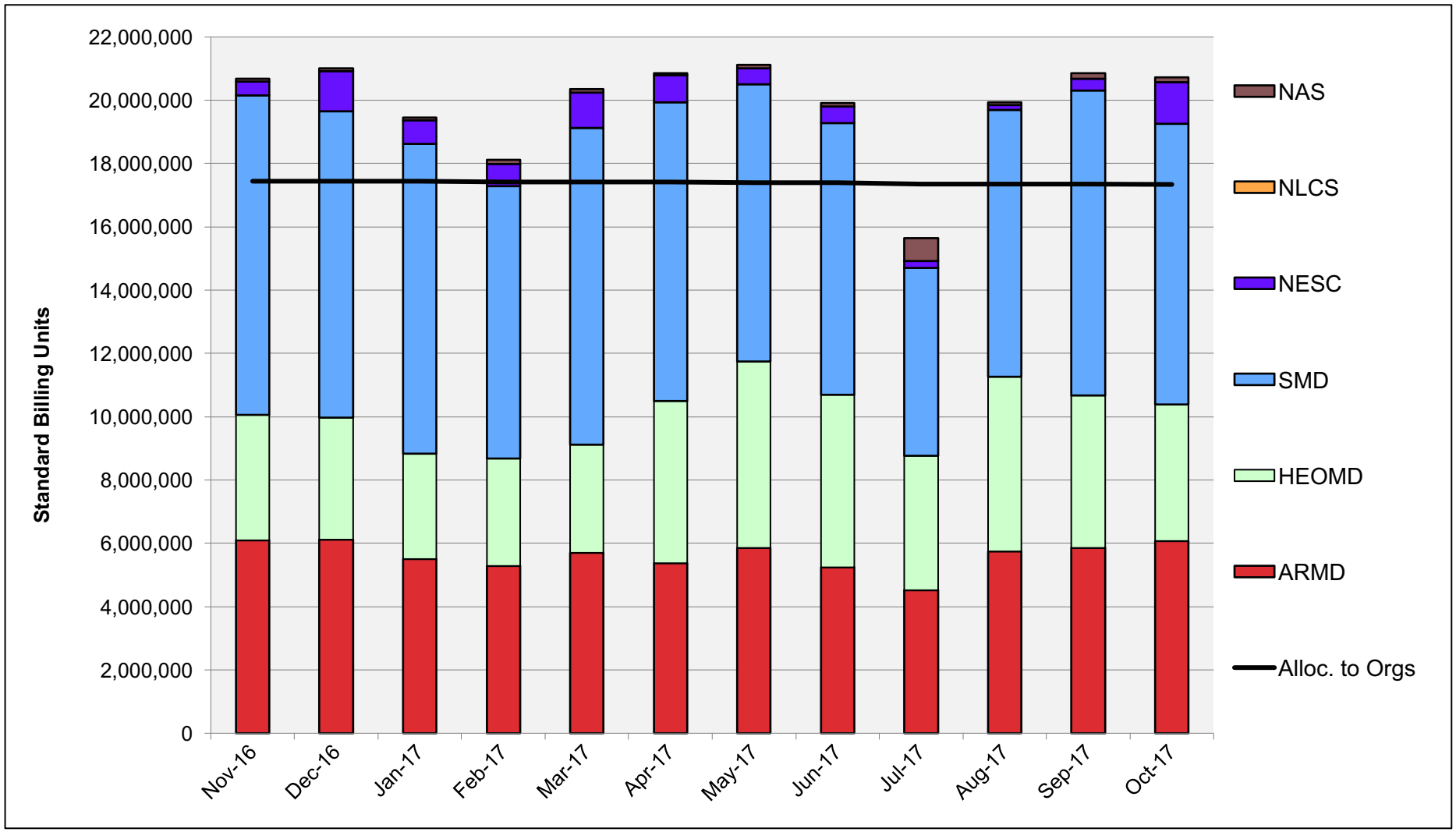
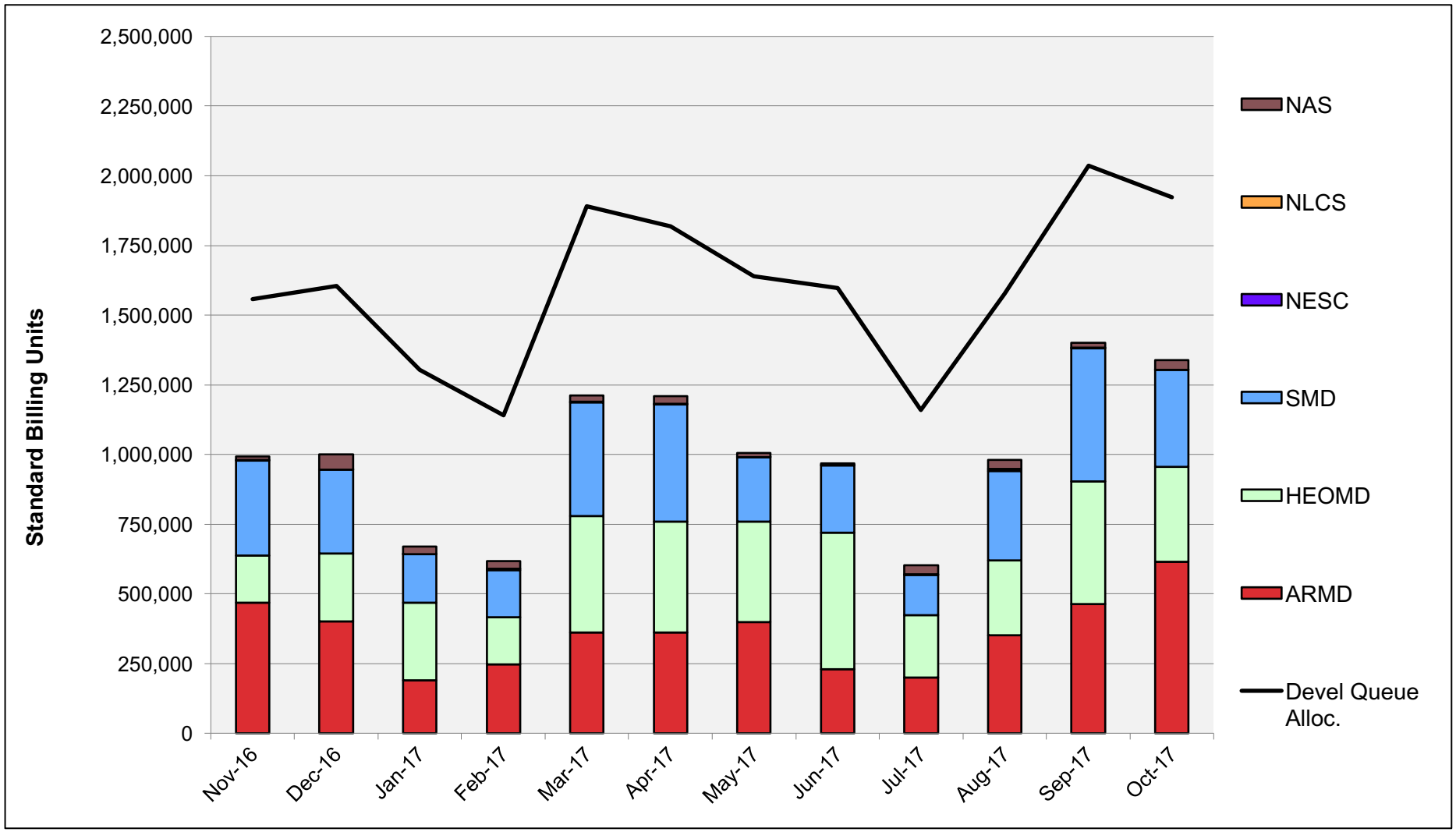


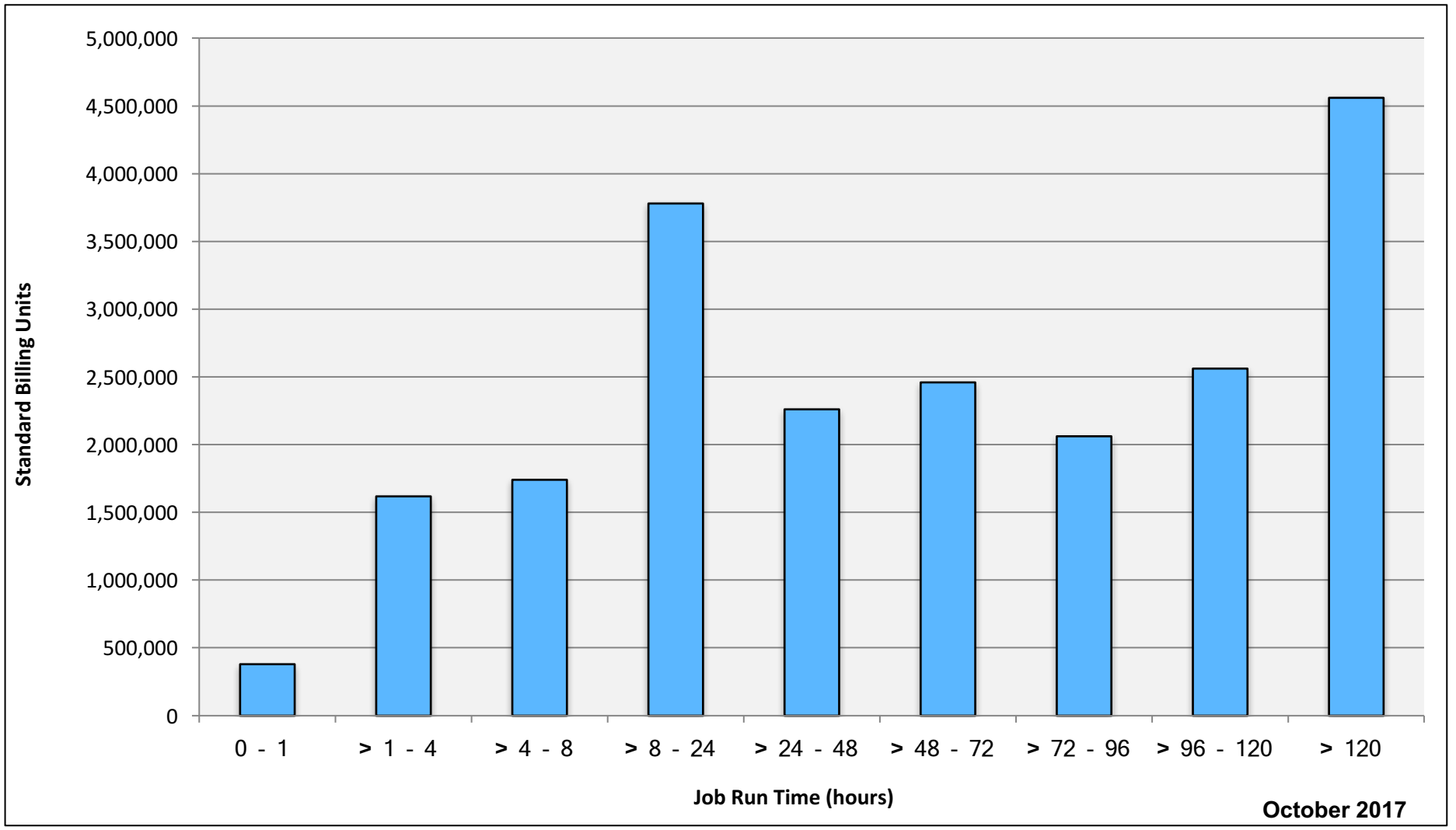
Pleiades:
SBUs Reported, Normalized to 30-Day Month



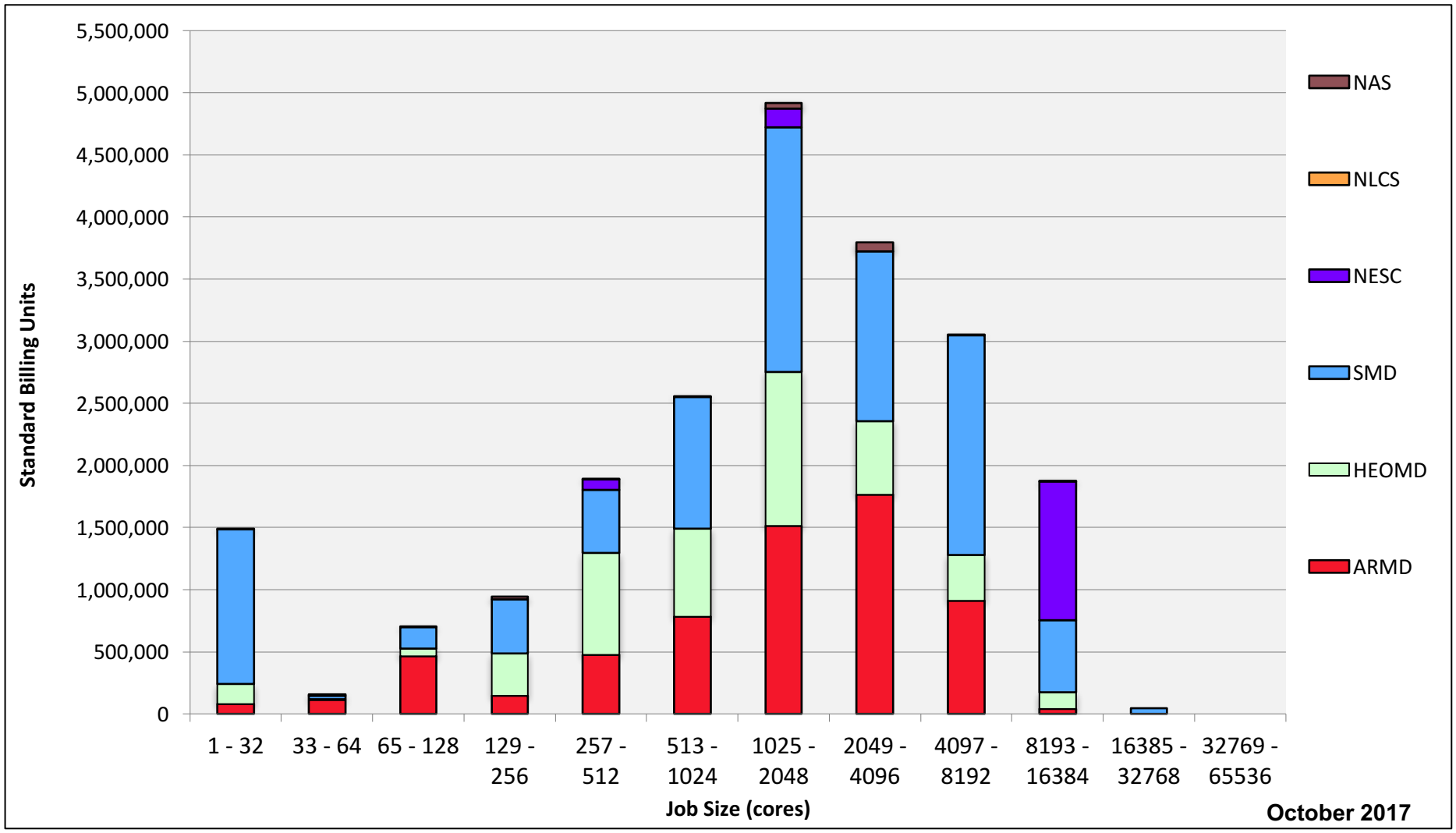
Pleiades:
Devel Queue Utilization



Pleiades:
Monthly Utilization by Job Length



Pleiades:
Monthly Utilization by Size and Mission



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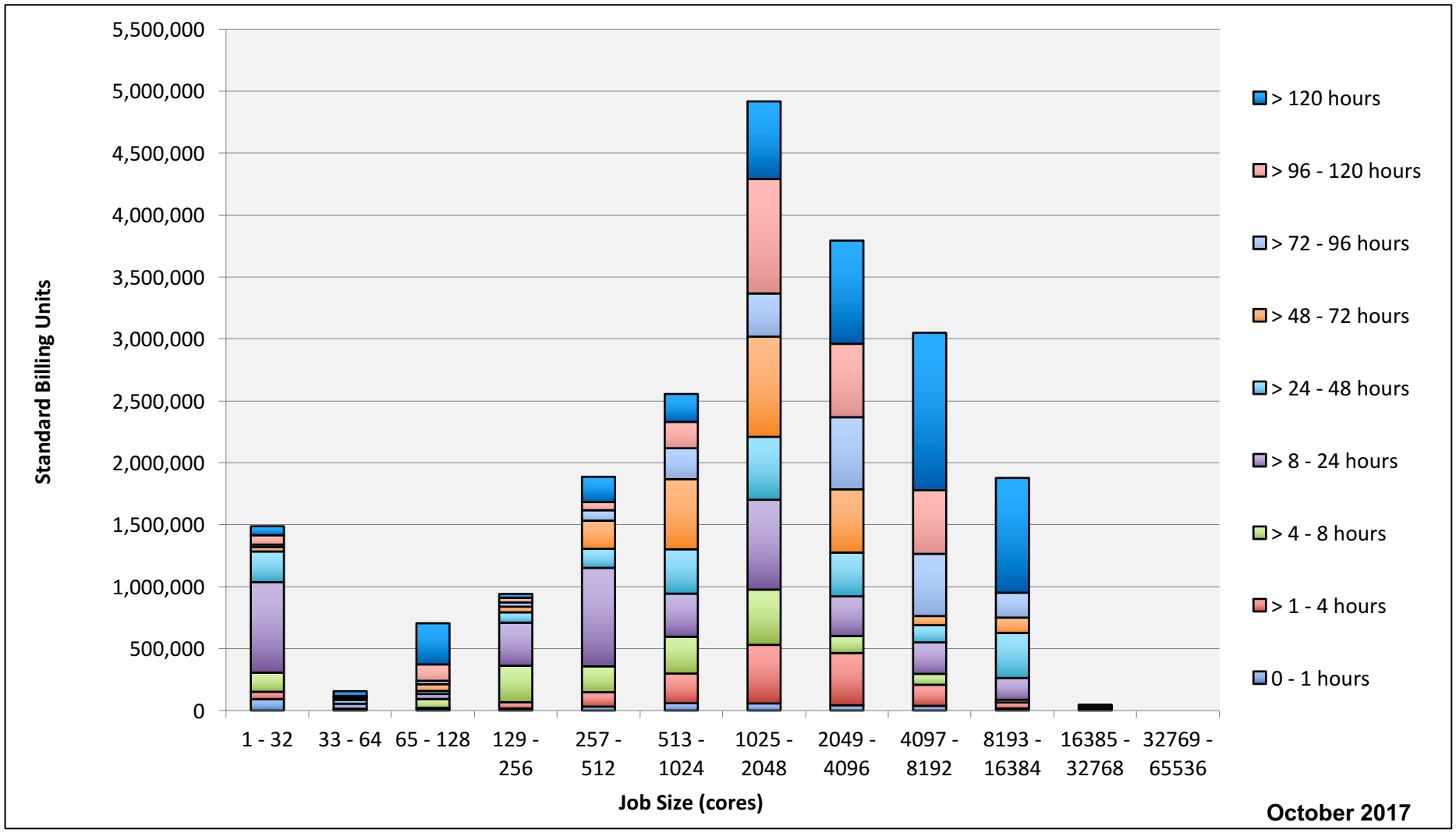
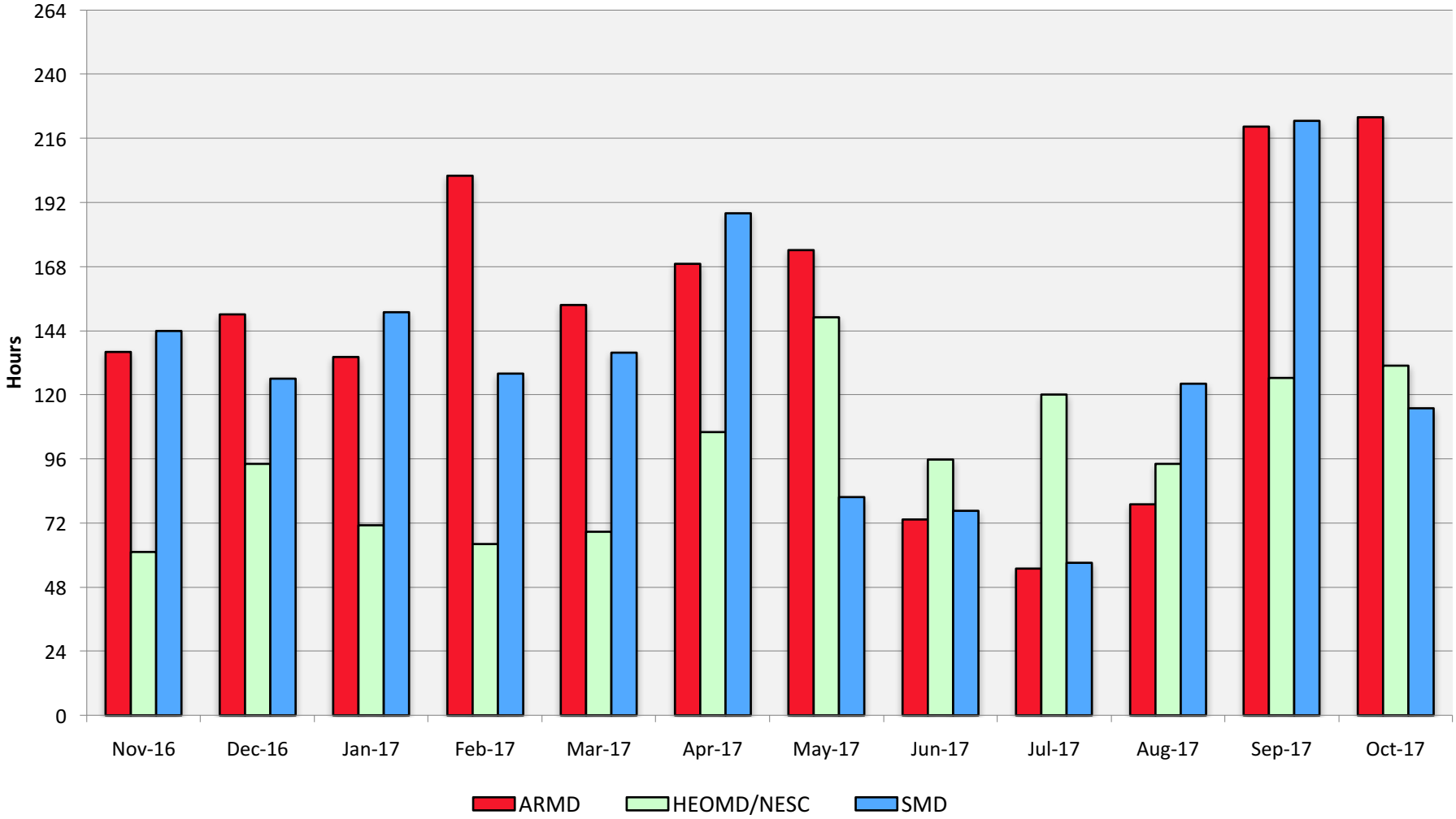
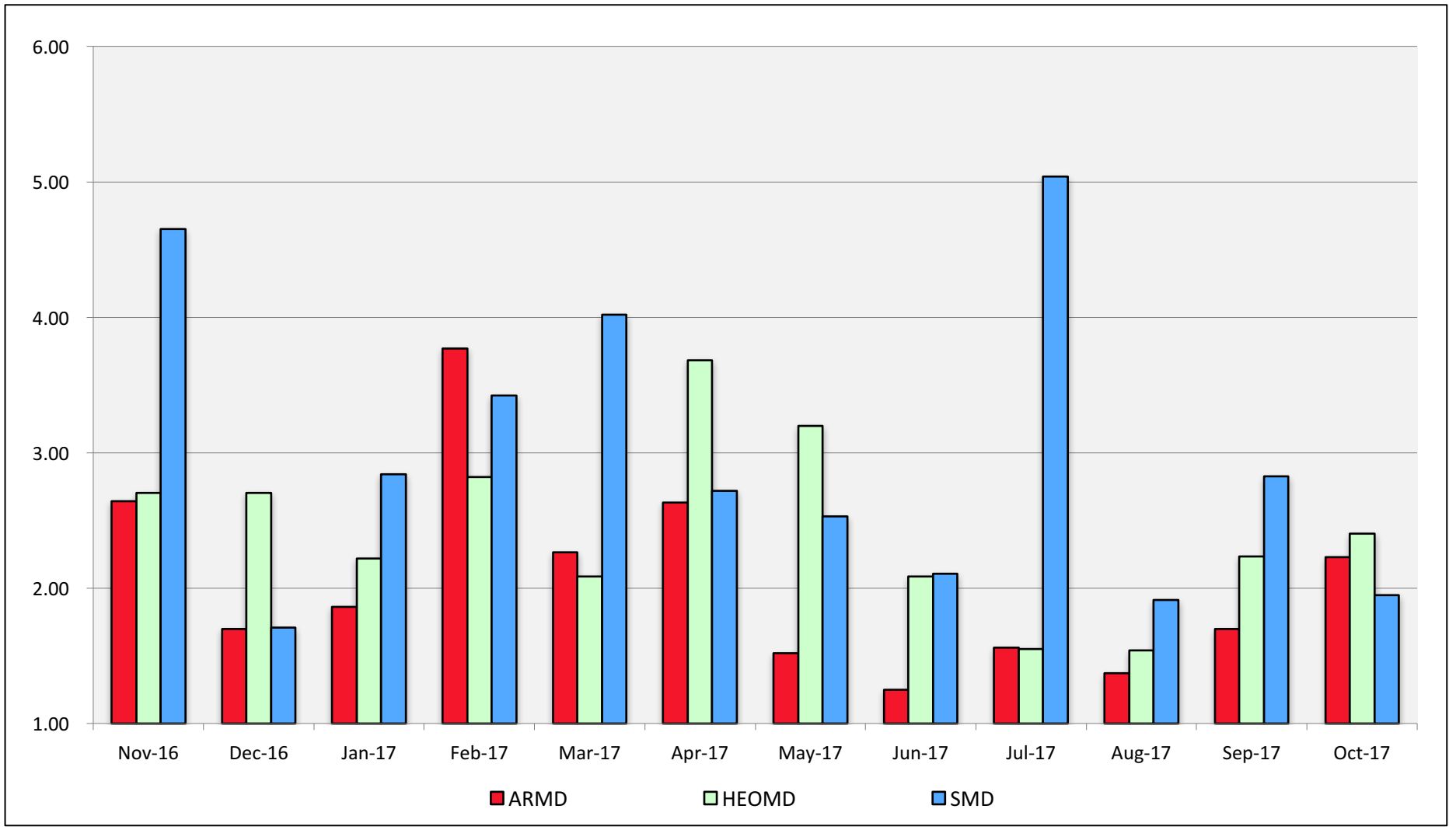


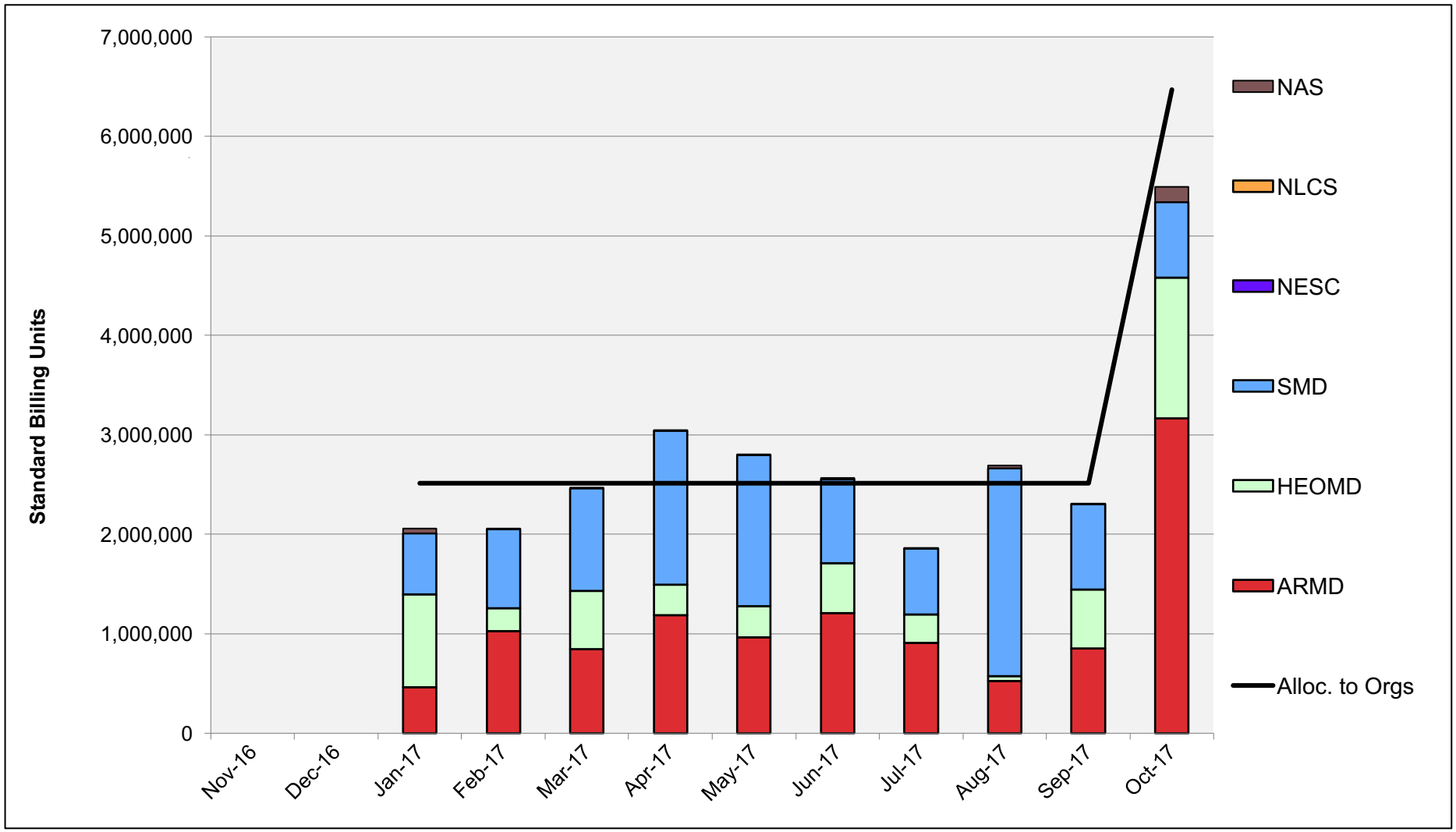
Pleiades:
Average Time to Clear All Jobs



Pleiades:
Average Expansion Factor



Electra:
SBUs Reported, Normalized to 30-Day Month



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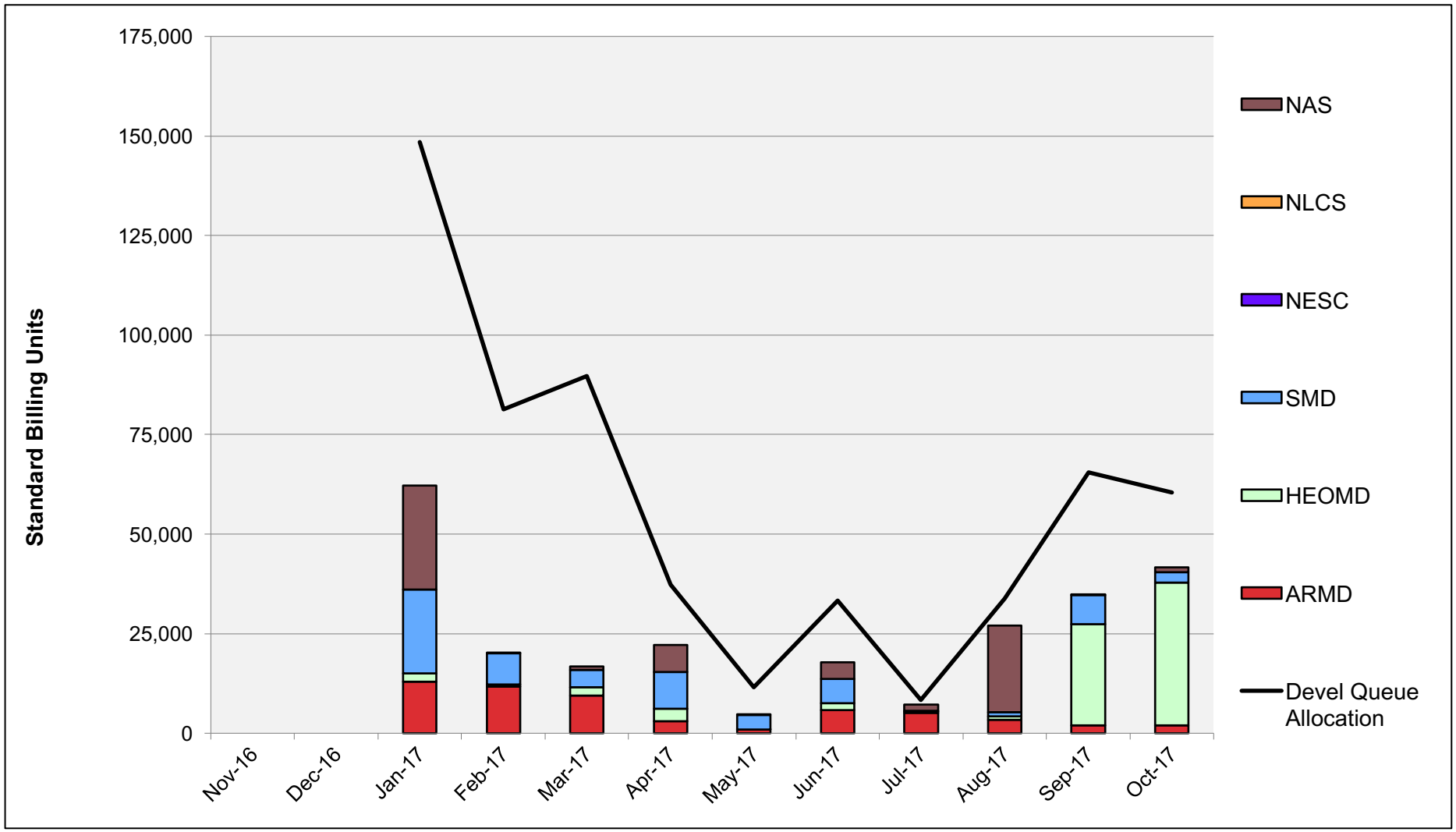
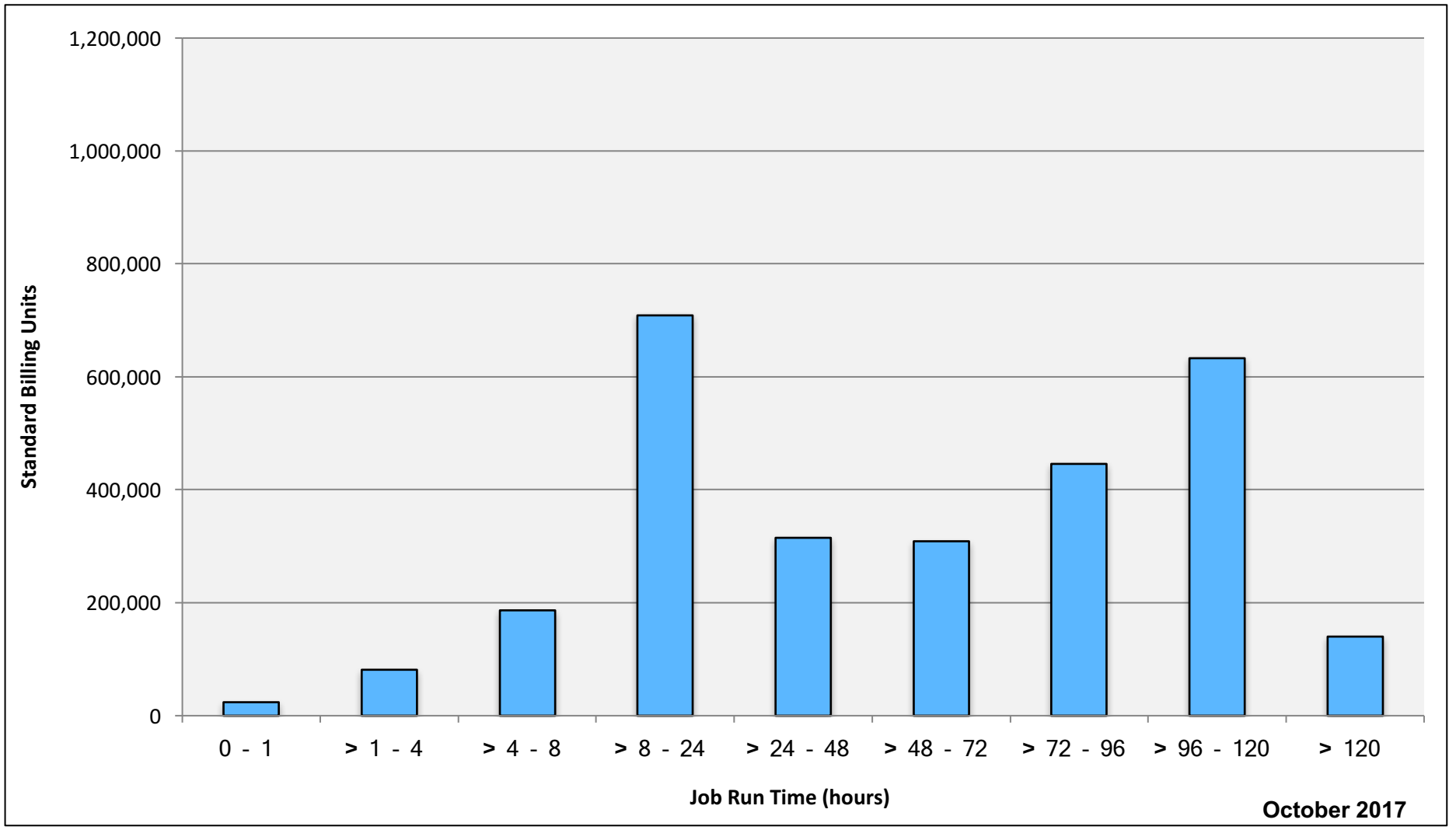
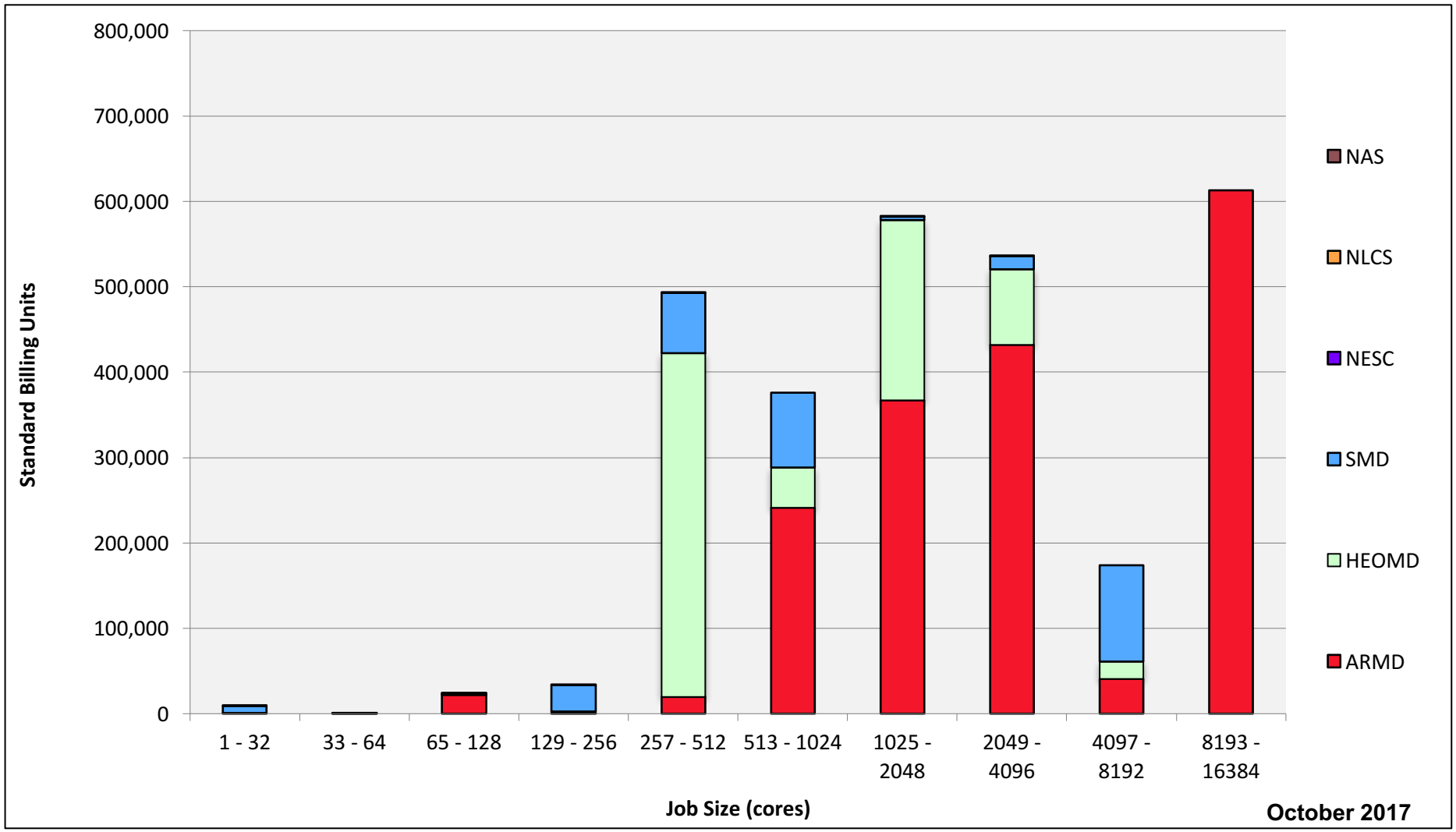
Devel Queue Utilization



Electra:
Monthly Utilization by Job Length



Electra:
Monthly Utilization by Size and Mission



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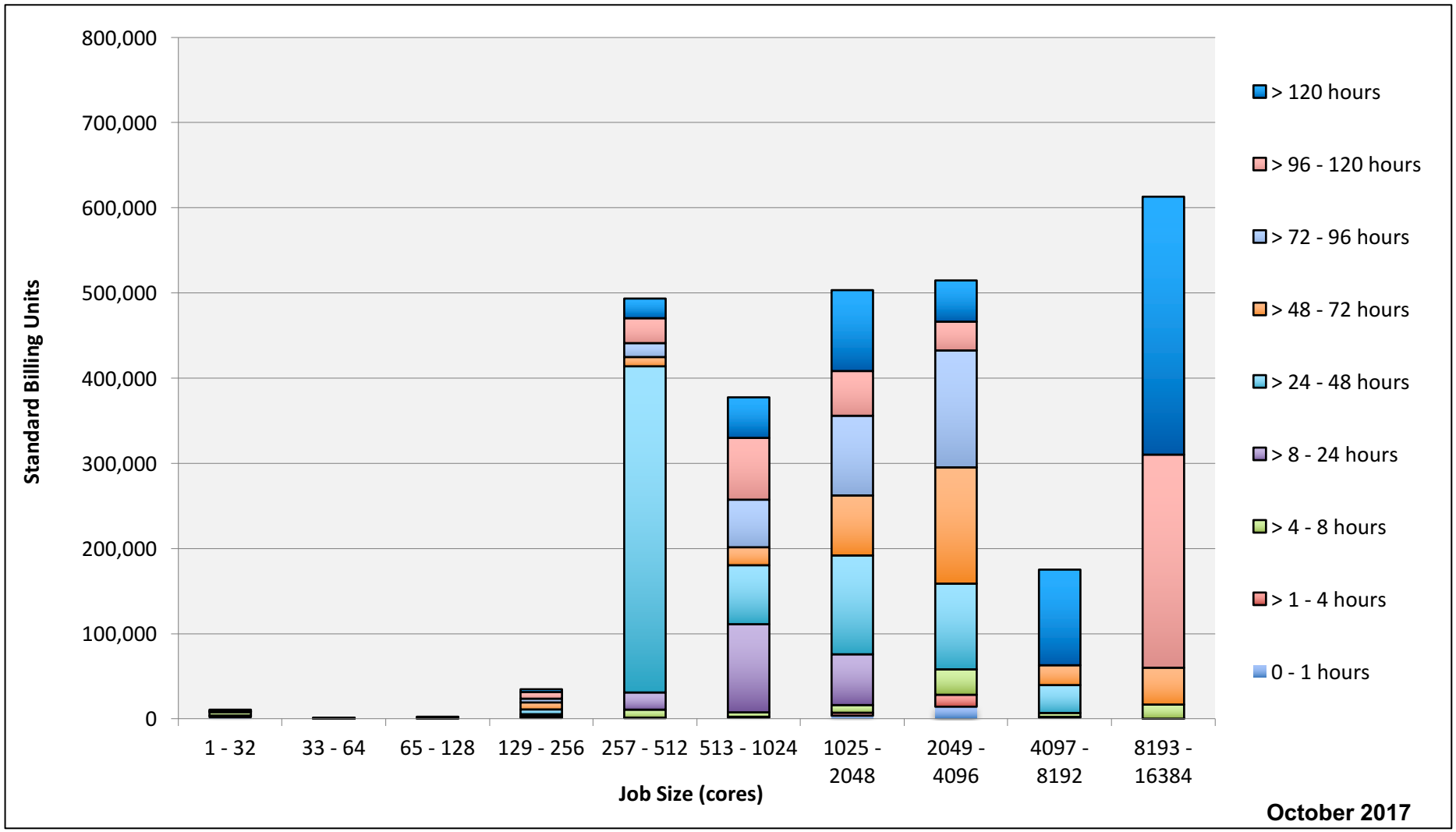
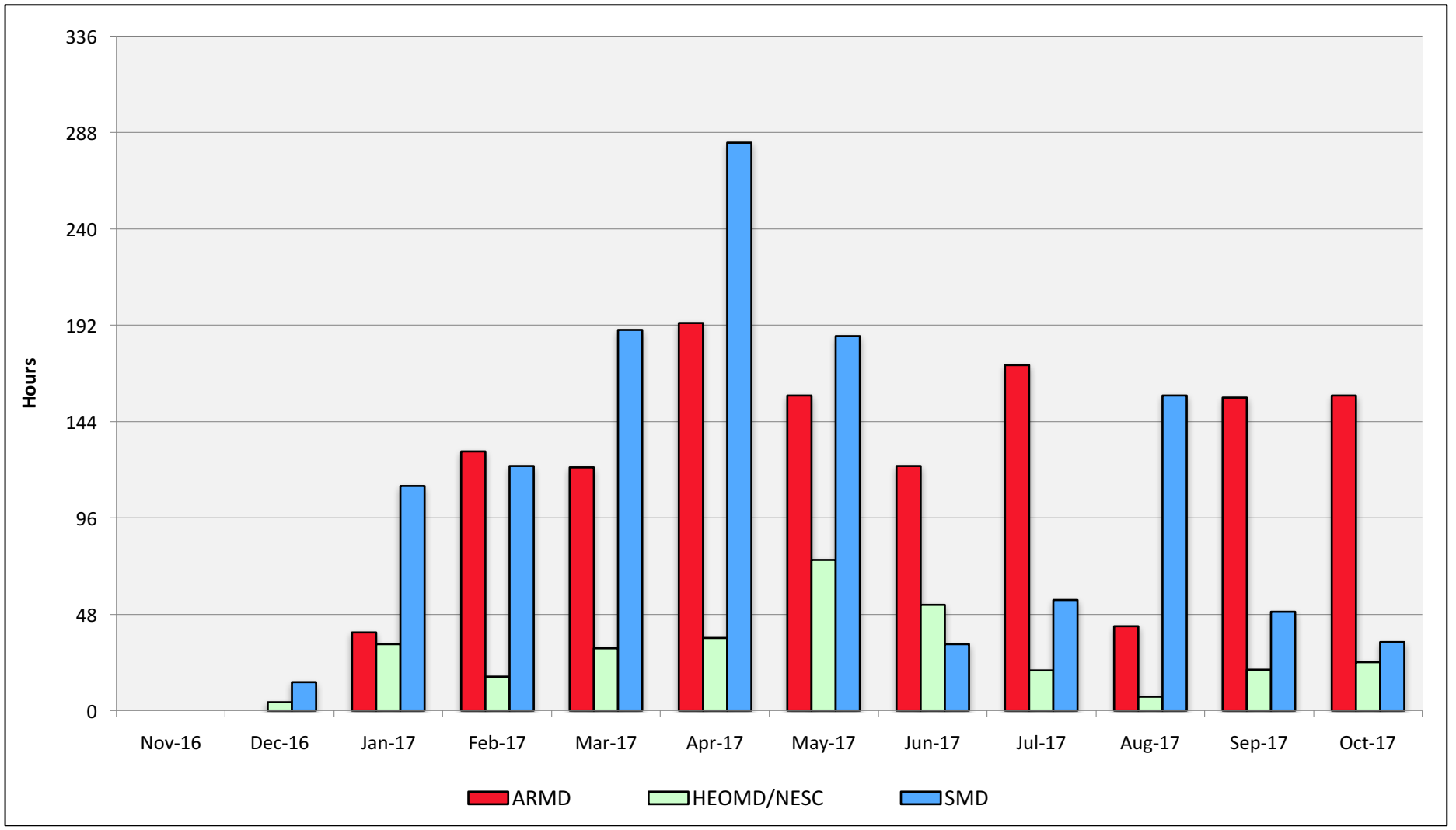
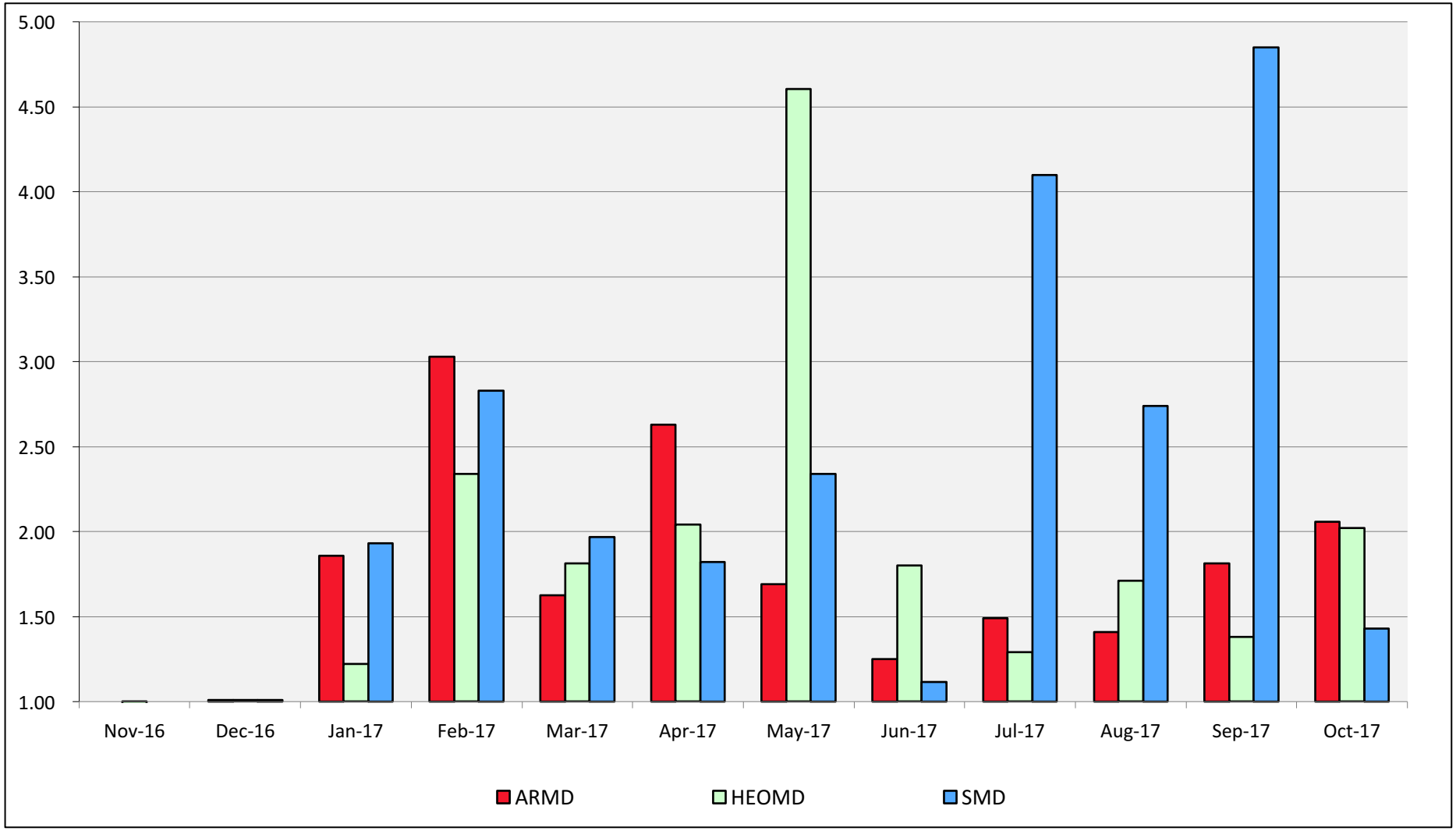
Monthly Utilization by Size and Length



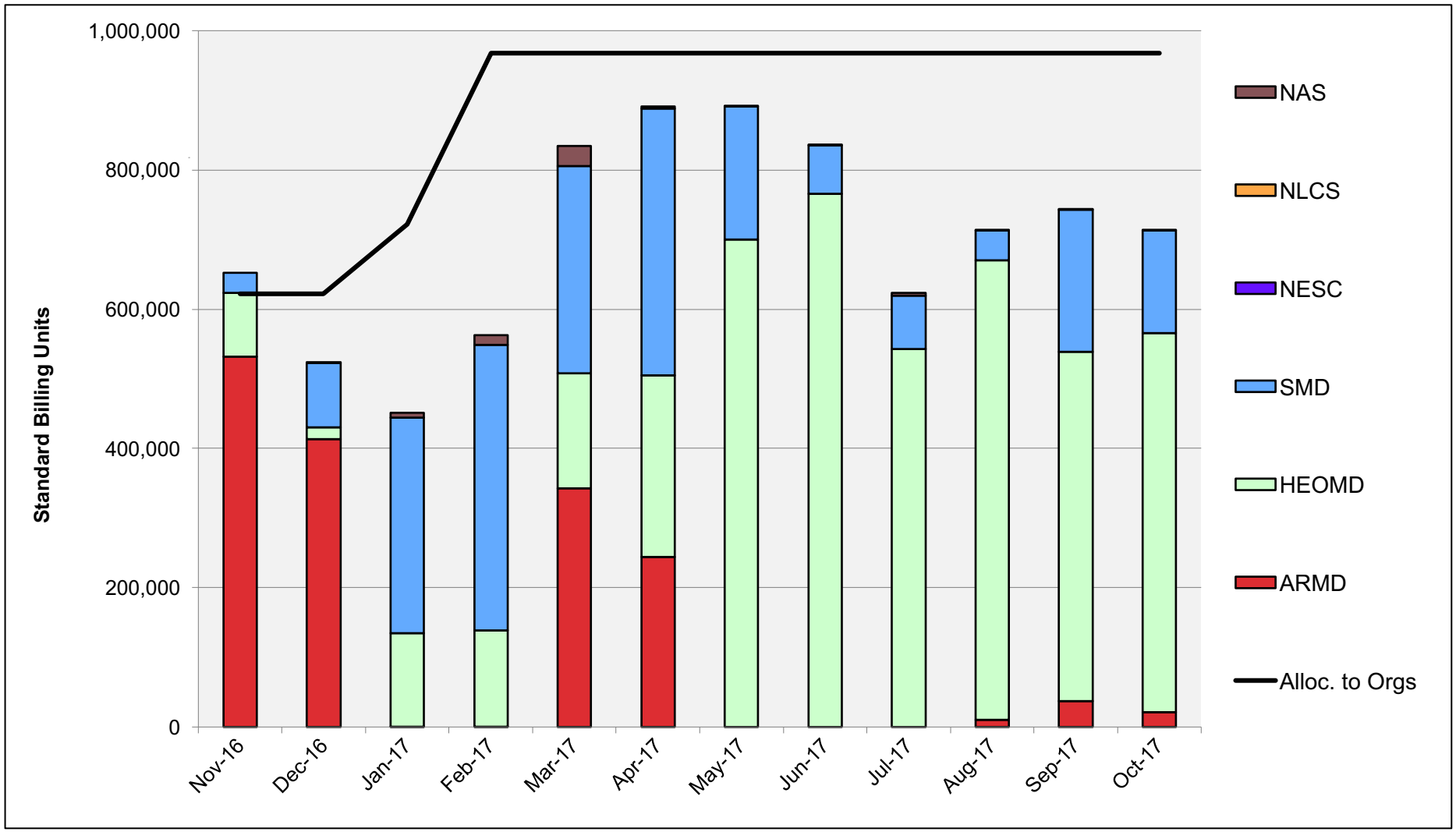
Electra:
Average Time to Clear All Jobs



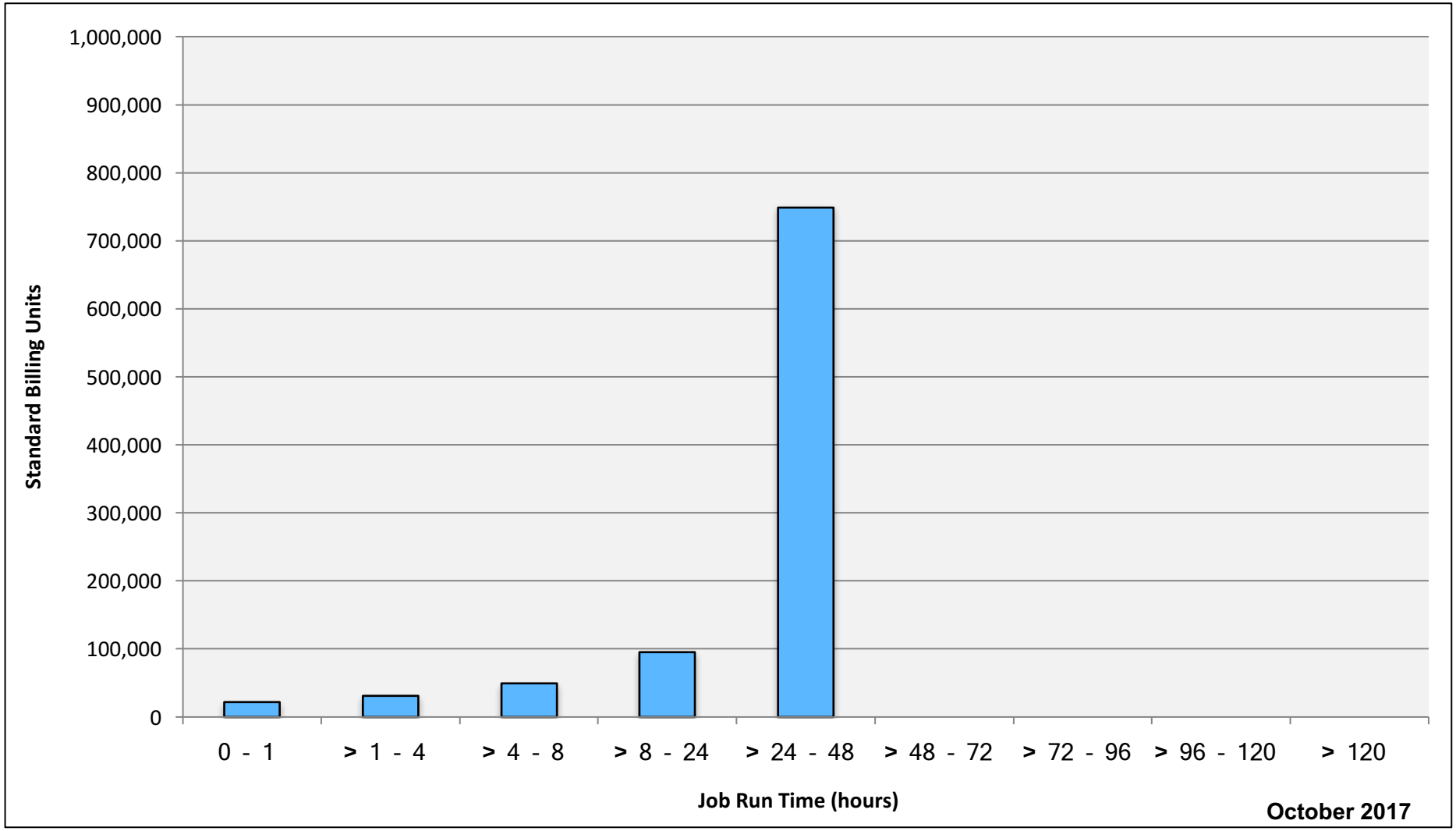
Electra:
Average Expansion Factor



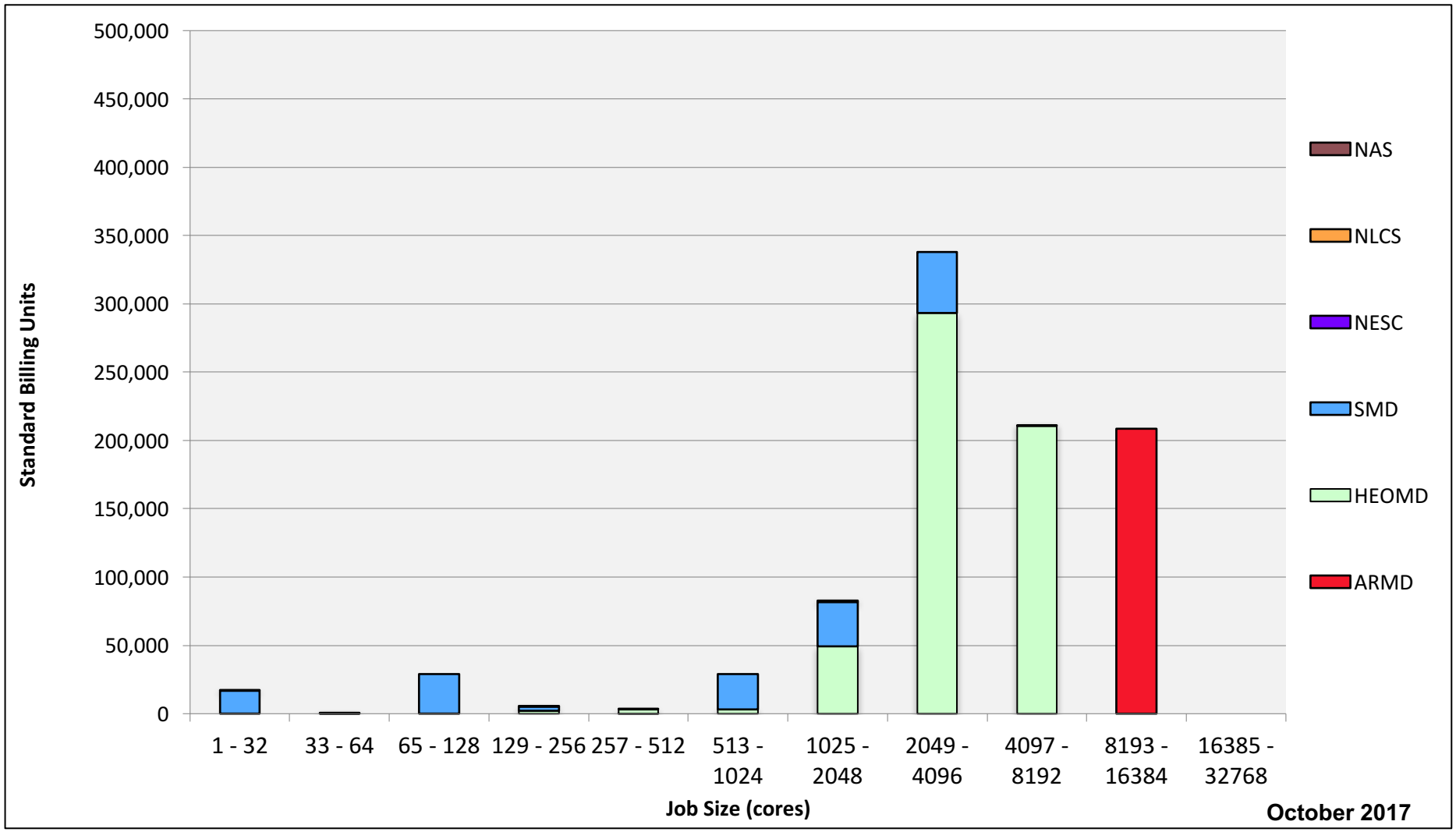
Merope:
SBUs Reported, Normalized to 30-Day Month



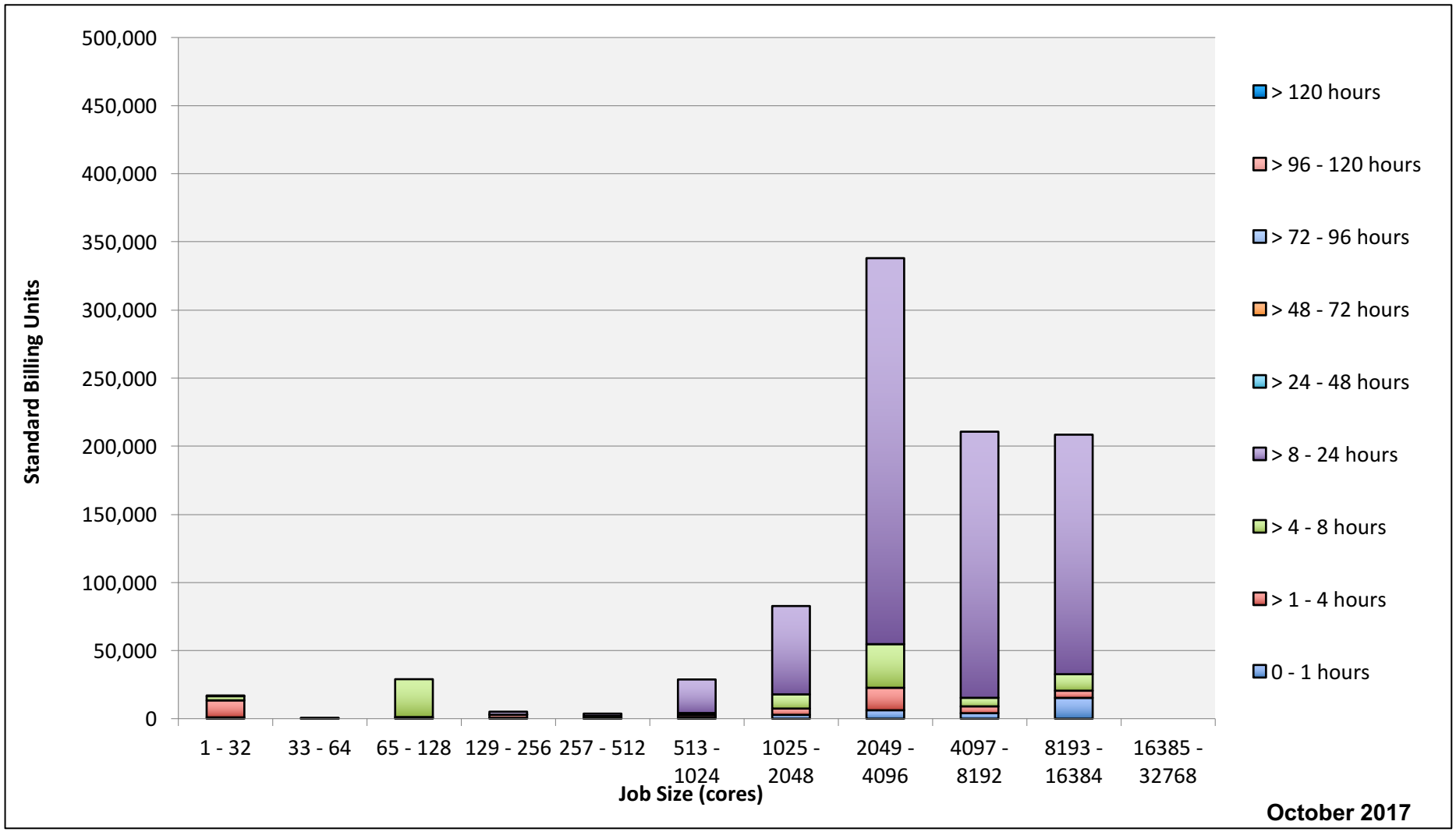
Merope:
Monthly Utilization by Job Length



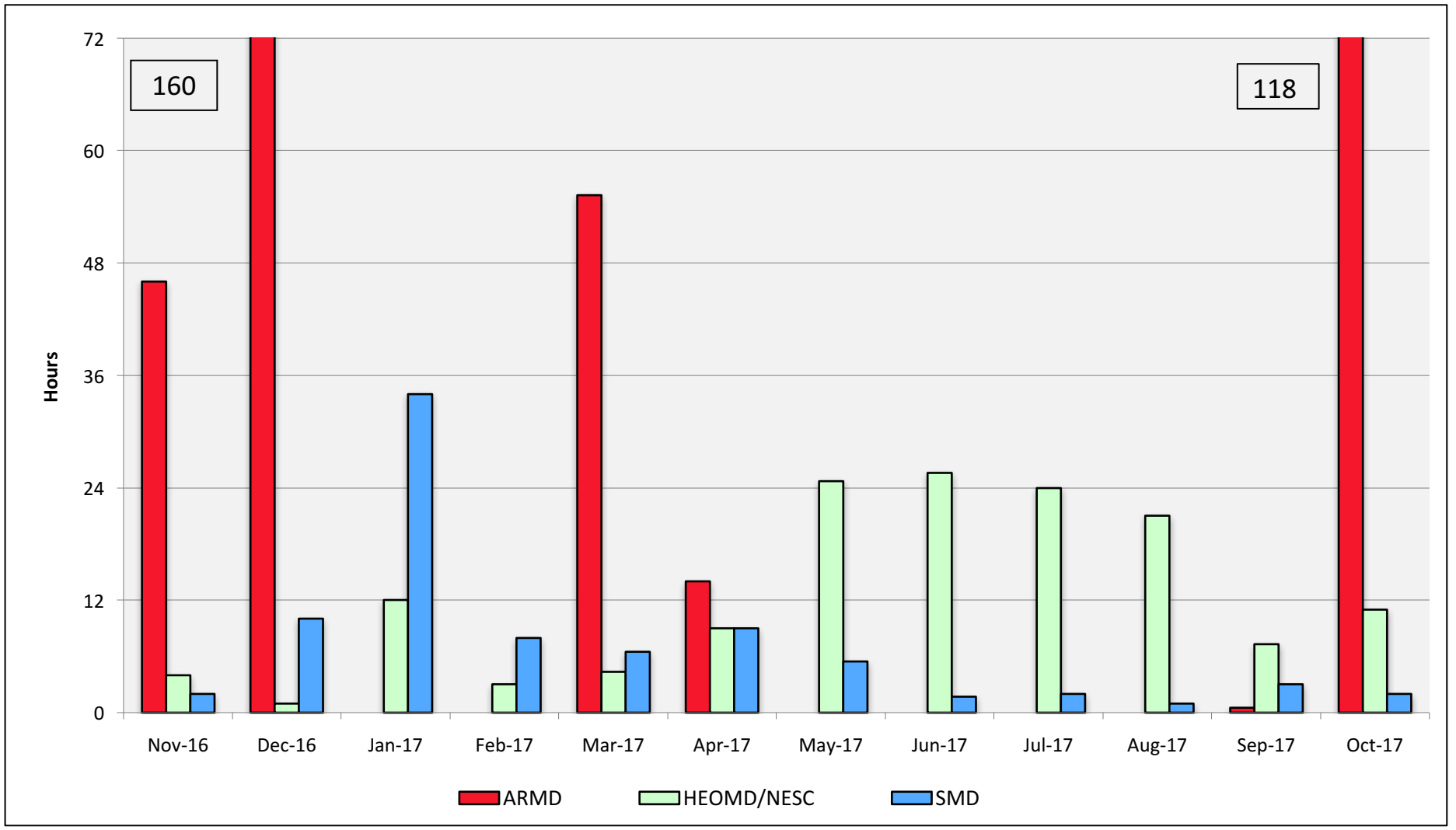
Merope:
Monthly Utilization by Size and Mission



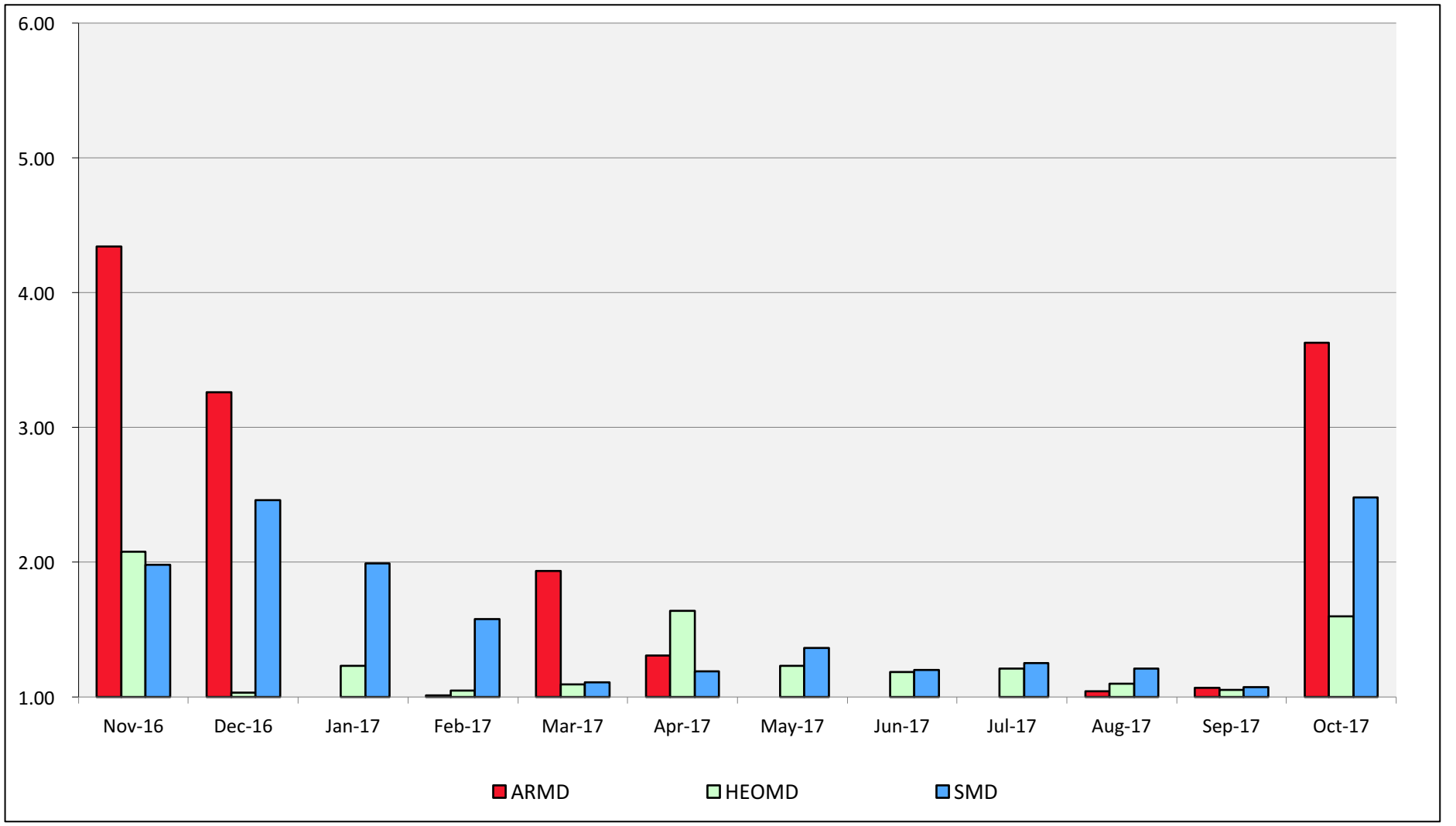
Merope:
Monthly Utilization by Size and Length



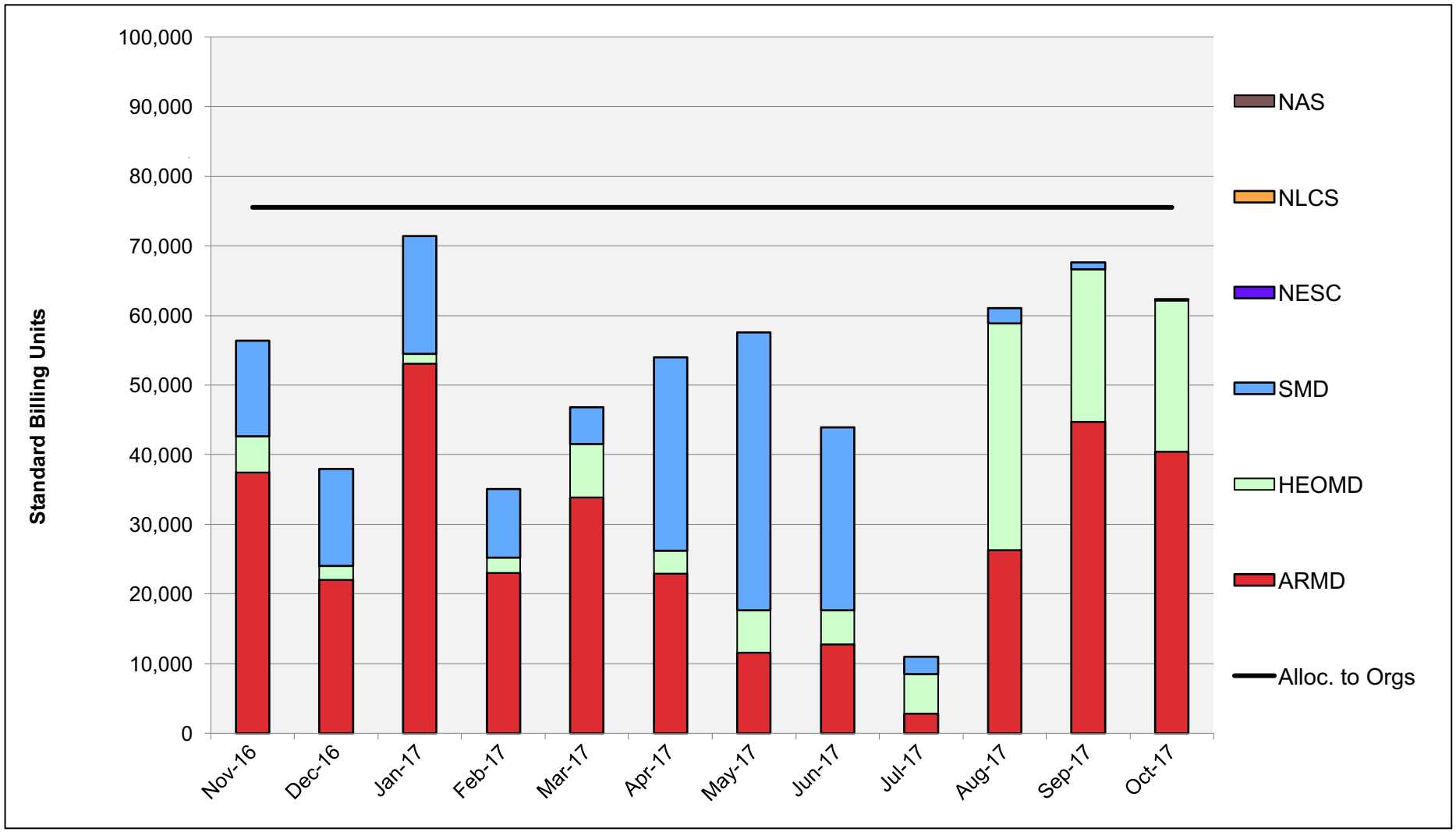
Merope:
Average Time to Clear All Jobs



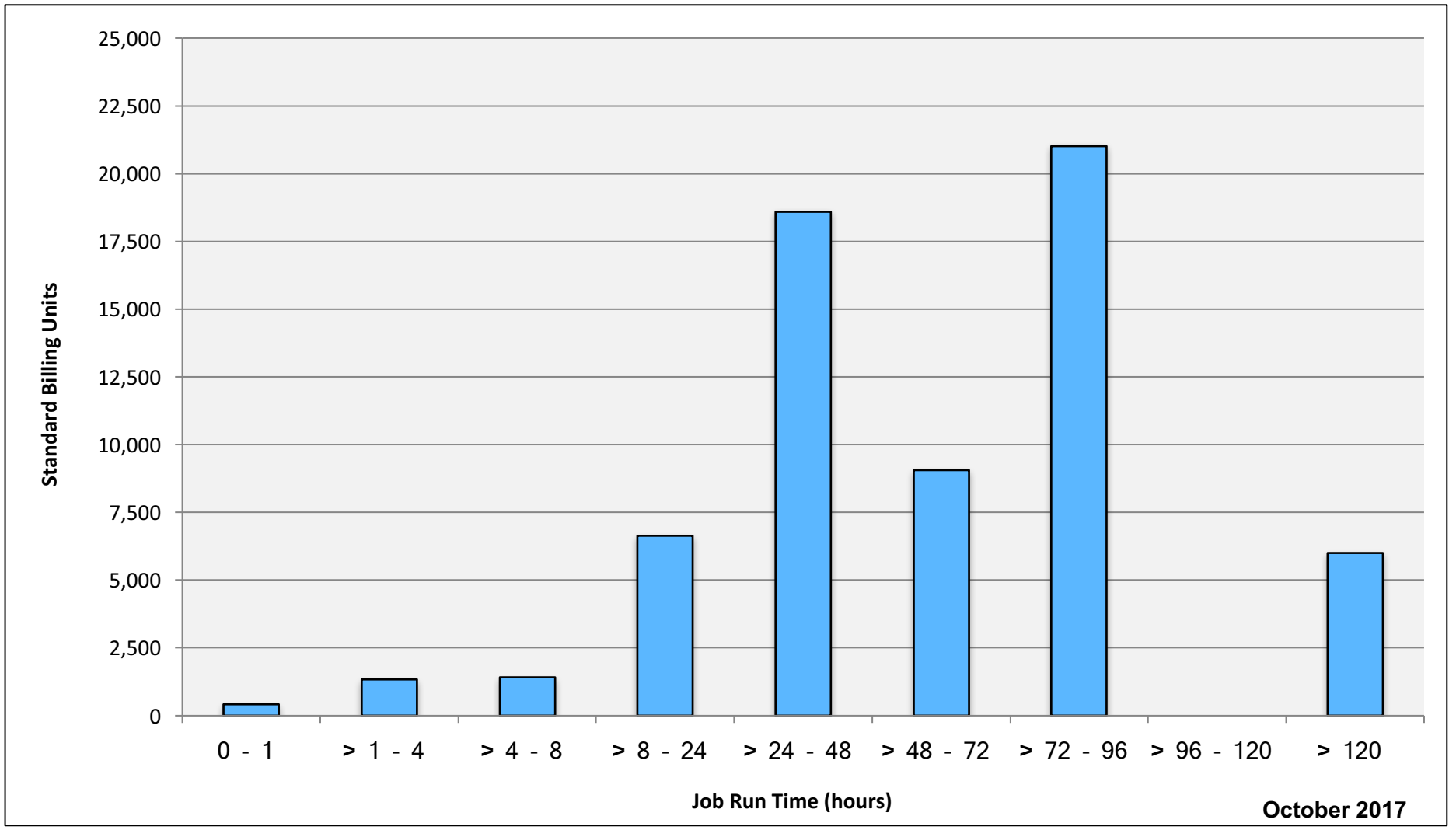
Merope:
Average Expansion Factor



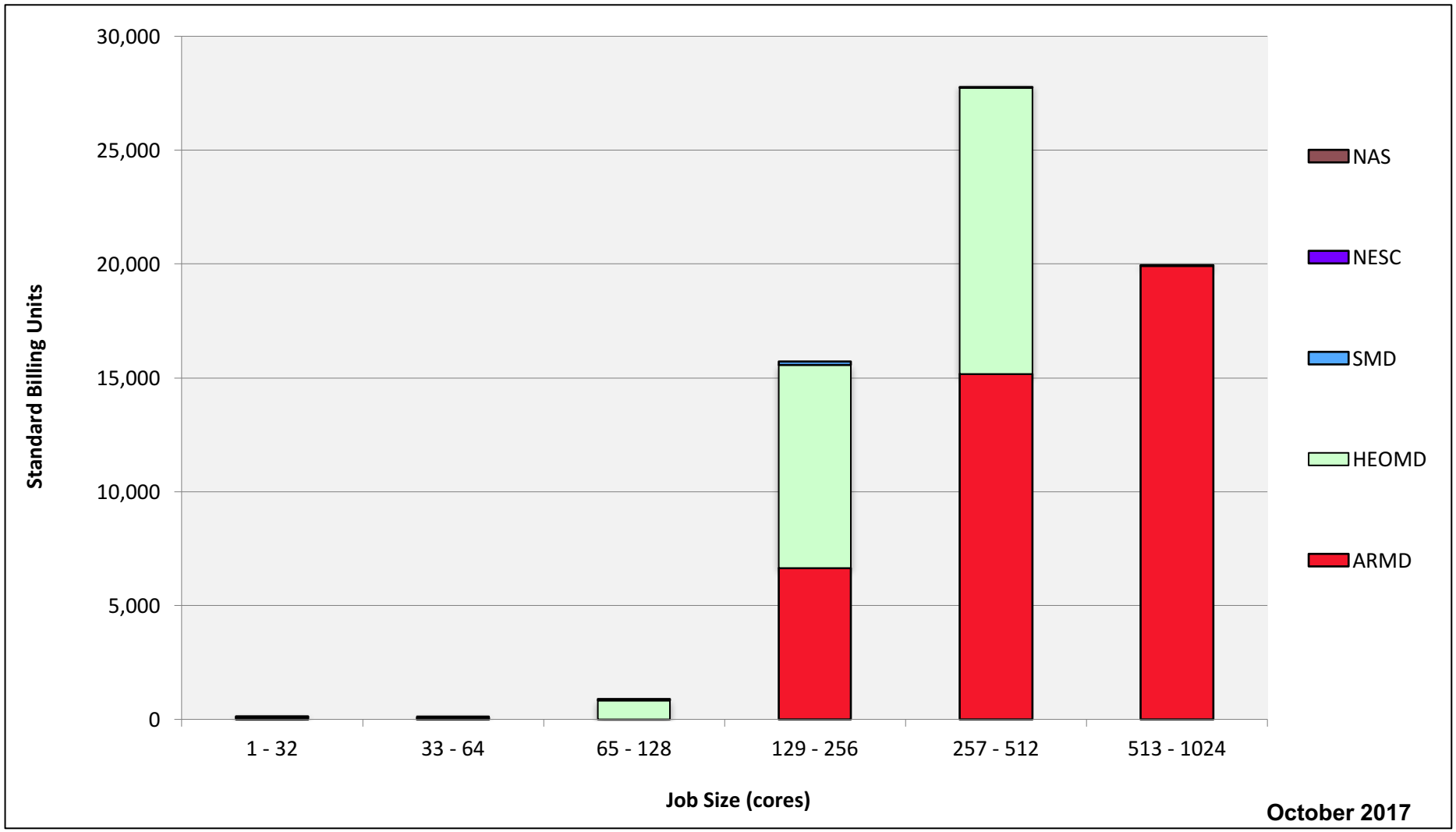
Endeavour:
SBUs Reported, Normalized to 30-Day Month



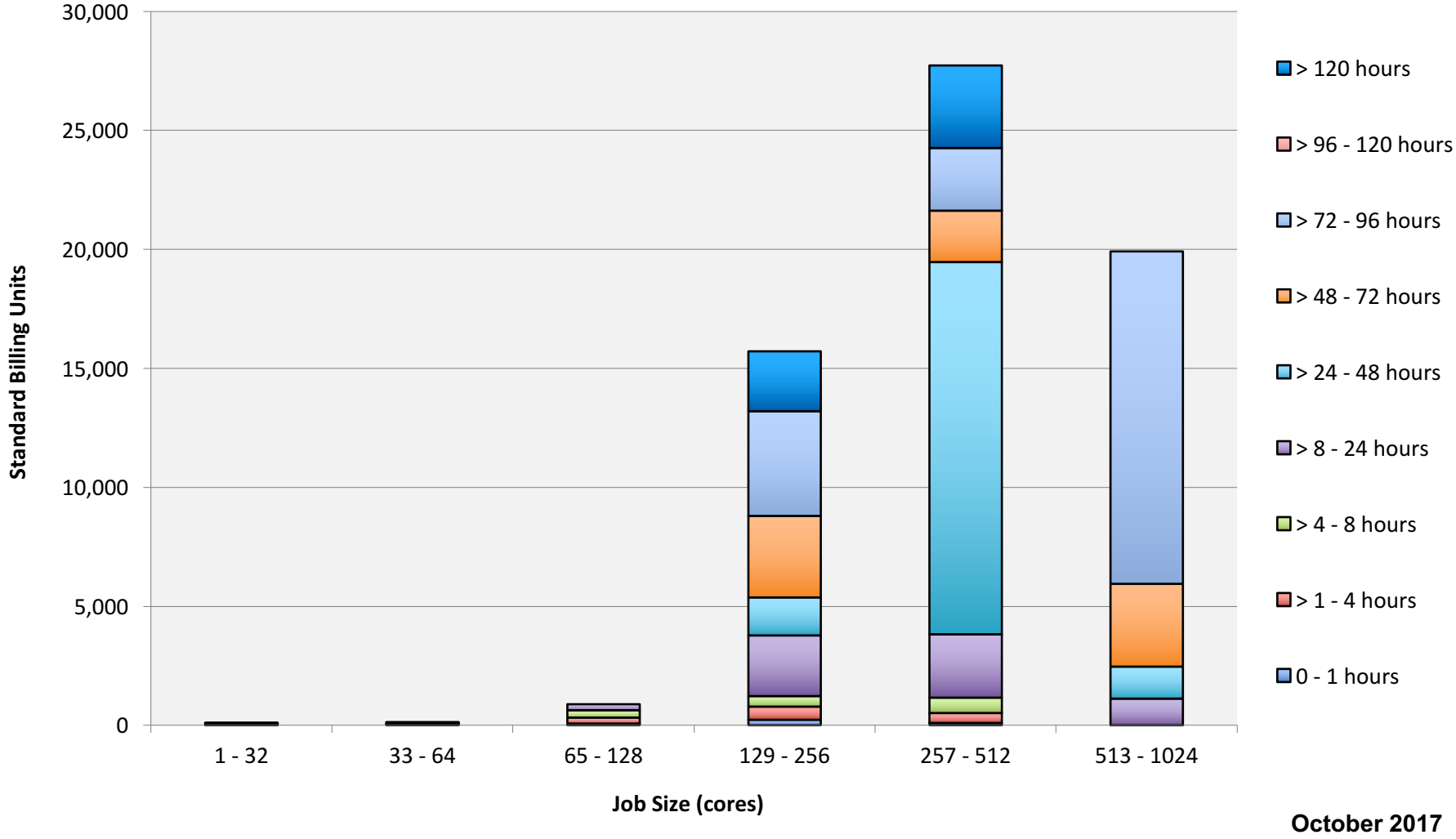
Endeavour:
Monthly Utilization by Job Length



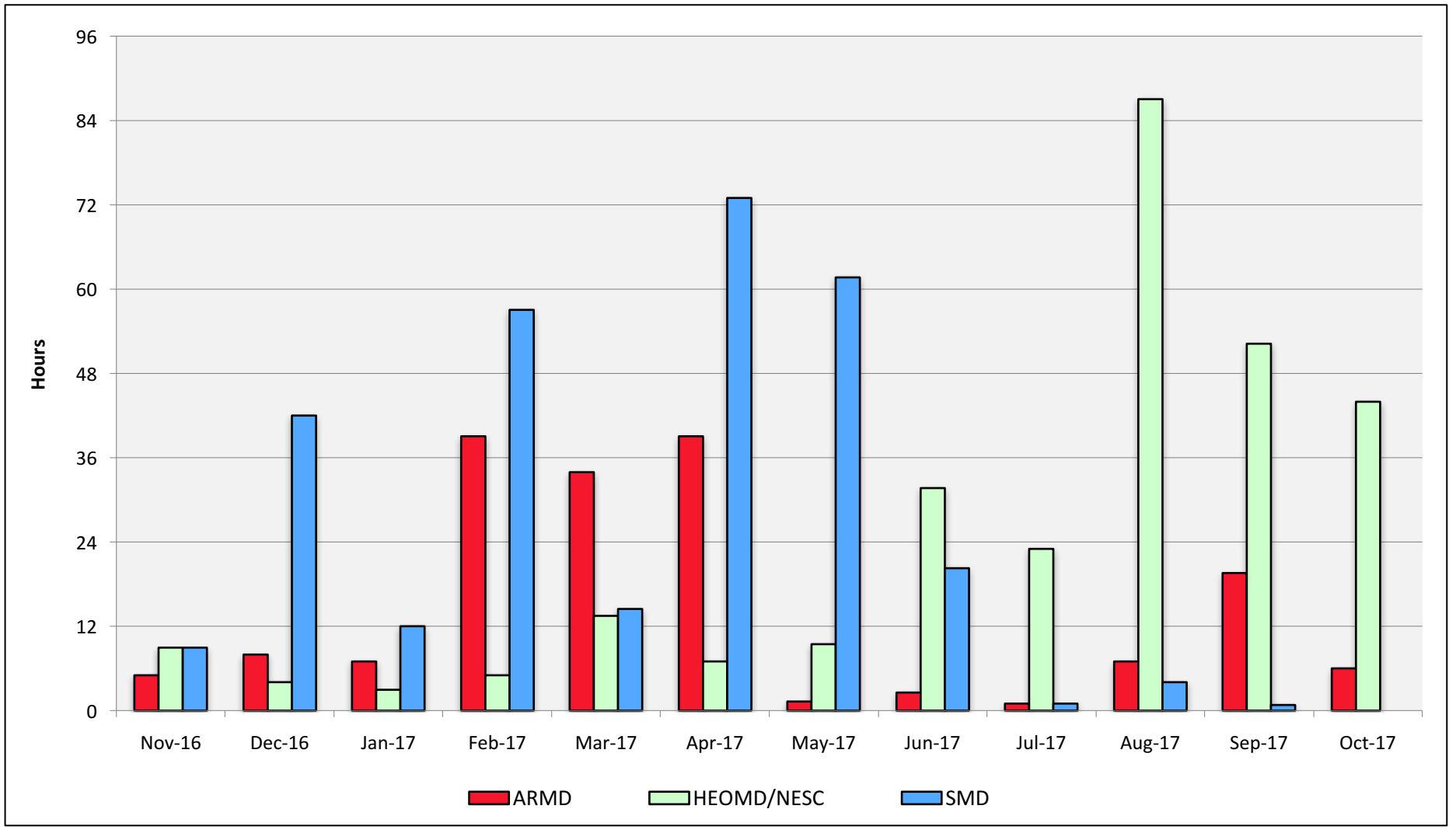
Endeavour:
Monthly Utilization by Size and Mission



Endeavour:
Monthly Utilization by Size and Length



Endeavour:
Average Time to Clear All Jobs



Endeavour:
Average Expansion Factor