Project Status Report

High End Computing Capability

Strategic Capabilities Assets Program

November 10, 2018

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Electra Supercomputer Expanded to 8.32 Petaflops

- HECC engineers completed the expansion of the Electra supercomputer, bringing the system's theoretical peak performance to 8.32 petaflops (PF).
- The expansion, comprising two Skylake E-cells with 576 compute nodes, was integrated in less than 1.5 weeks from equipment delivery. The quick deployment was made possible by extended installation support from the vendor, Hewlett Packard Enterprise (HPE).
- After the expansion was completed, the HECC Systems and APP teams performed extensive benchmarking and diagnostics to stress-test the entire Electra system prior to releasing the new configuration to users.
- The Modular Supercomputing Facility is now at maximum capacity with the Broadwell and Skylake nodes, and maximum power usage of 1.64 megawatts.

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

The Electra supercomputer is configured with 1,152 Broadwell nodes and 2,304 Skylake nodes in two modular containers, with a combined Power Utilization Efficiency (PUE) rating of approximately 1.03—reported averages for data centers around the world range from 1.8–2.5 PUE.

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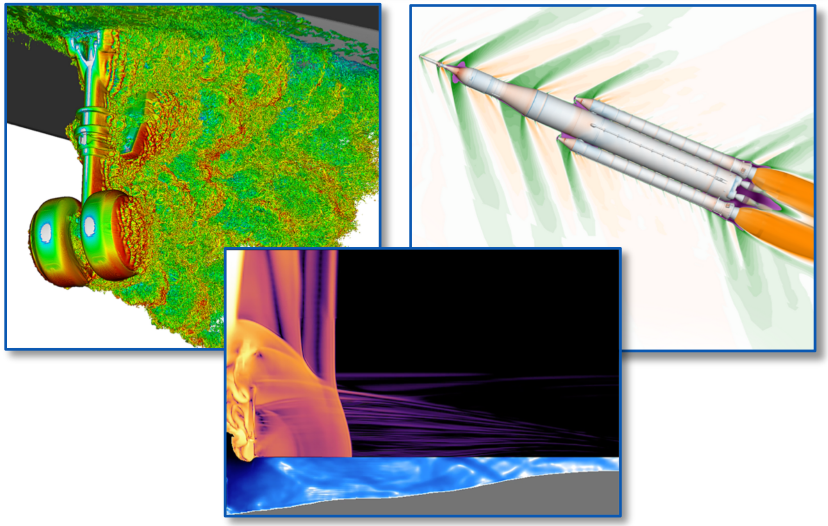
Chris Buchanan, chris.buchanan@nasa.gov, (650) 604-4308,
NASA Advanced Supercomputing Division, ASRC

New Allocation Period for Supercomputer Time Begins for NASA Mission Directorates

- The new allocation period for all NASA mission directorates began October 1.
- All allocations were converted to the new Broadwell-based Standard Billing Unit (SBU)* rate, which went into effect on October 1.
- The mission directorates awarded about 97 million SBUs (roughly 381 million SBUs at the previous rate) to 484 projects.
- The Aeronautics Mission Directorate (ARMD) awarded over 34 million SBUs to 148 projects.
- The Human Exploration and Operations Mission Directorate (HEOMD) awarded nearly 28.5 million SBUs to 75 projects.
- The Science Mission Directorate (SMD) awarded over 34 million SBUs to 261 projects.
  - SMD awarded roughly 92% of its share, as it will be phasing awards during the coming year. This is a 20% increase compared to the previous 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.



Images representing the variety of projects supported by HECC resources. Clockwise from top left: 1) Simulation of landing gear noise using the Launch, Ascent and Vehicle Aerodynamics (LAVA) Cartesian Lattice-Boltzmann discretization. *Michael Barad, Joseph Kocheemoolayil, NASA/Ames;* 2) Space Launch System Block 1 vehicle ascent flow field, simulated using NASA's OVERFLOW code. *Derek Dalle, Henry Lee, NASA/Ames;* 3) Simulation of tsunami and blast waves generated by the impact of a 1-gigaton, 100-meter diameter iron asteroid into the ocean, produced with the ALE3D hydrocode. *Darrel Robertson, NASA/Ames.*

POC: Emily Kuhse, emily.kuhse@nasa.gov, (650) 604-1687, NASA Advanced Supercomputing Division, ASRC

**1 SBU equals 1 hour of a Pleiades Broadwell 28-core node.*

SBU Benchmarking on NCCS Skylake Cluster Leads to Improvement on Electra

- When evaluating the differences in the SBU rates for Skylake-based nodes at NAS and NCCS, HECC's Application Performance and Productivity (APP) team found that the boot configurations of the supercomputers at the two locations were different. Subsequent changes to Electra improved its performance by an average of 1.3%.
  - Skylake nodes on Electra and Discover are largely identical. The main difference is that Electra uses InfiniBand for its interconnect while Discover uses OmniPath.
  - The APP team previously ran the SBU benchmark suite on the Skylake portions of Electra and Discover and found rates of 1.59 and 1.61, respectively.
  - APP staff initially attributed the ~1% variance in SBU performance to the different interconnect technologies. However, follow-up testing showed that Discover was faster on single-node benchmarks, especially if cores were left idle. They quickly determined there were differences in settings of the TurboBoost feature, which under some conditions is able to increase processor clock rates.
- Working with HECC's Systems team, APP staff tested different TurboBoost settings on Electra. The settings chosen improved the performance of DGEMM—the double-precision matrix-matrix multiplication routine—by 40% when run with one core on each socket. Other applications, run on sparsely-populated Skylake nodes, saw a 5–10% performance boost.

Mission Impact: By benchmarking performance on external machines, HECC is able to validate that its resources are performing as expected, thereby maximizing their effectiveness for HECC users.

One-node benchmarks, such as matrix-matrix multiply, were used to help determine the cause of performance differences between Skylake-based nodes on the Electra system at NASA Ames and those on the Discover system at NASA Goddard. There are 288 nodes in an HPE E-cell (pictured).

POCs: Johnny Chang, johnny.chang@nasa.gov, (650) 604-4356, Dale Talcott, dale.r.talcott@nasa.gov, (650) 604-0555, NASA Advanced Supercomputing (NAS) Division, ASRC

Tools Team Implements New HECC SBU Rate Accounting Changes

- The SBU rate change introduced many required changes to accounting scripts, databases, and reports. The HECC Tools team inventoried all scripts and web applications that currently compute SBU rates. Scripts were identified for updating, in order to discontinue using hard-coded values.
- A dry run was performed two weeks prior to the go-live date of the new SBU values to verify and fix any issues.
- MicroStrategy update times were reduced from two weeks to less than 30 minutes due to code improvements that resulted in only six components to change, as opposed to more than 90 changes in past iterations.
- The Tools team updated report templates to reflect the SBU change across historic data, making the rates consistent across reports.

Mission Impact: The NASA Standard Billing Unit (SBU), based on Broadwell architecture, is a way of standardizing work across dissimilar architectures. The new SBU definition helps users understand the underlying computer architecture and true cost of computation—leading to more effective use of resources.

	Skylake	Broadwell	Haswell	Ivy Bridge	Sandy Bridge	Westmere
SBU2 (Current)	1.59	1	0.8	0.66	0.47	0.29
SBU1 (Retired)	6.43	4.04	3.34	2.52	1.82	1
Change in Cost	-3%	-3%	-6%	3%	2%	14%

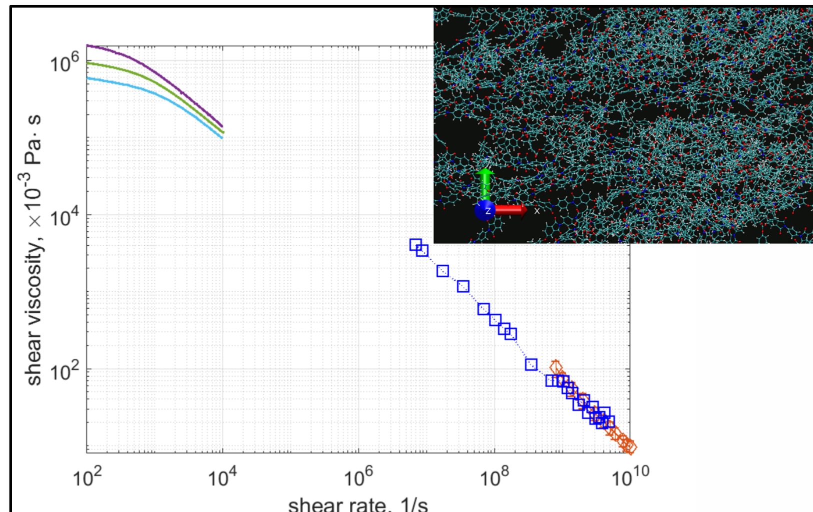
This chart reflects the change from Westmere-based Standard Billing Units (SBUs) to Broadwell-based SBUs.

POC: Blaise Hartman, blaise.hartman@nasa.gov, (650) 604-2539, NASA Advanced Supercomputing Division

Cloud-Based Computing Enables Realistic 3D Aerospace Manufacturing Simulations

- Materials scientists working on optimizing 3D manufacturing for aerospace applications have narrowed the gap between experiment and simulation by using cloud-based resources.
  - As part of the HECC project to test mechanisms for accessing commercial clouds, the scientists used GPU-accelerated nodes from Amazon Web Services (AWS) to analyze the strength of polymer-polymer interfaces with molecular dynamics (MD) simulations.
  - They improved the accuracy of atomistically informed predictions, narrowing the gap between predictions from MD simulations and experimental data by more than 2 orders of magnitude.
  - Previously, the researchers performed coarse-grained approximations using the LAMMPS MD code running without GPUs, shown as red squares in the graph at right. Their new fine-grained simulations, which used the GROMACS MD package running on GPUs, are indicated by blue squares in the graph.
  - They found HECC's environment for bursting to AWS cloud resources to be stable and easy to use.
- The researchers plan to extend these results to predict other important aerospace manufacturing parameters, paving the way for exploration of novel frontiers in nanomanufacturing.

Mission Impact: HECC's pilot cloud-bursting mechanism provided scientists access to NVIDIA Tesla K80 GPUs in the cloud, allowing them to narrow the gap between experiment and simulation in aerospace manufacturing.



This graph shows atomistically resolved molecular dynamics (MD) predictions of the shear viscosity for flat polymer-polymer interfaces as squares at lower right. These can be compared with experimental data on bulk samples at upper left. The inset shows MD predictions obtained on the Pleiades supercomputer.

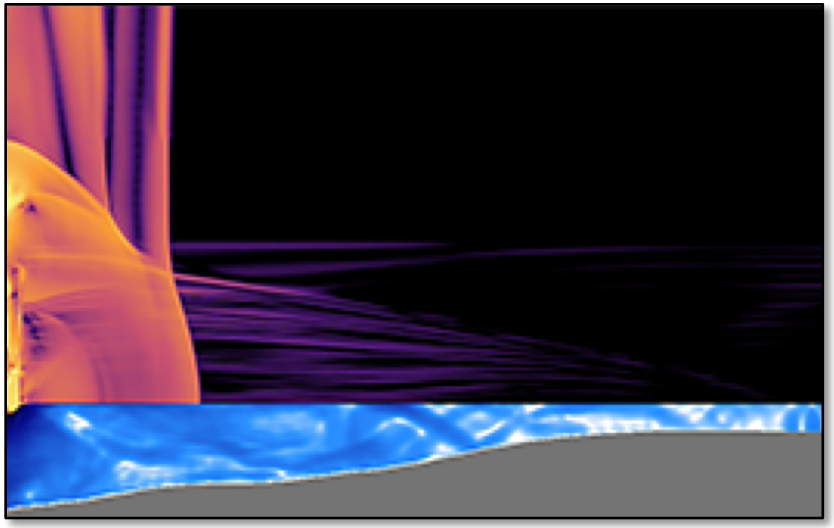
POCs: Dmitry Luchinsky, dmitry.g.luchinsky@nasa.gov, (650) 604-2330, Intelligent Systems Division, SGT, Inc.; Gabriele Jost, gabriele.jost@nasa.gov, (650) 604-0468, NASA Advanced Supercomputing Division, Supersmith

Pleiades Enables Millions of Asteroid Impact Cases for Risk Assessment*

- Researchers working on the Asteroid Threat Assessment Project (ATAP) at NASA Ames are running simulations on Pleiades to efficiently analyze millions of impact scenarios from asteroids of various sizes and properties.
- The ATAP-developed Probabilistic Asteroid Impact Risk (PAIR) model samples from statistical distributions of asteroid properties, models the atmospheric entry and breakup of each case, and evaluates damage at locations around the world.
  - Results provided key data for NASA's 2017 Near-Earth Objects Definition (NEO) Science Definition Team (STD) study to help reevaluate which asteroid sizes pose enough threat to warrant tracking.
  - The NEO STD study required 60 million impact cases, run in parallel on 1,600 cores, to produce converged results across the broad size range considered.
  - PAIR is also at-the-ready to evaluate damage risks along specific impact corridors if a potential asteroid threat is discovered.
- PAIR results have supported several impact exercises in which NASA, FEMA, DOE, and other groups use hypothetical impact scenarios to prepare for how to evaluate and respond to such a threat.

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

Mission Impact: HECC supercomputing resources enable high-fidelity simulations that are essential to studying the complex processes involved in asteroid atmospheric entry, impact, and the resulting hazards.



Snapshot from a simulation of tsunami and blast waves generated just after impact of a 1-gigaton, 100-meter diameter iron asteroid into the ocean, produced with the ALE3D hydrocode. Blue contours show water velocities; orange show the velocity of air pressure waves emanating from the vertical entry column of water rebounding up from the initial impact cavity and the surface impact. *Darrel Robertson, NASA/Ames*

POCs: Lorien Wheeler, lorien.wheeler@nasa.gov, (650) 604-0785, NASA Advanced Supercomputing (NAS) Division, ASRC; Donovan Mathias, donovan.mathias@nasa.gov, (650) 604-0836, NAS Division

HECC Facility Hosts Several Visitors and Tours in October 2018

- HECC hosted 5 tour groups in October; guests learned about the agency-wide missions being supported by HECC assets, and some groups also viewed the D-Wave 2000Q quantum computer system. Visitors this month included:
  - A delegation from the NATO Parliamentary Assembly, including officers of the Science and Technology Committee: Chairperson Maria Martens (Netherlands), Vice Chair Bruno Vitorino (Portugal), and General Rapporteur Susan Davis (United States); 15 countries were represented.
  - A large group from the Mission Support Directorate, who were at Ames for a Face-to-Face session; the tour included several deputy center directors and most associate center directors from other NASA centers.
  - Congressman Gerald Mark McNerney, U.S. Representative for California's 9th congressional district.
  - A large group from the U.S Department of Commerce International Delegation, Americas Competitive Exchange on Innovation and Entrepreneurship.

NASA Advanced Supercomputing Division Chief Piyush Mehrotra presents simulation results on the NASA hyperwall to NATO parliamentary delegation members.

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

Papers

- “**Turbulence Structure in a Stratocumulus Cloud**,” G. Matheou, Atmosphere, vol.9, issue 10, October 10, 2018. *
  https://www.mdpi.com/2073-4433/9/10/392
- “**The Role of Downflows in Establishing Solar Near-Surface Shear**,” L. Matilsky, B. Hindman, J. Toomre, arXiv:1810.00115 [astro-ph.SR], October 2, 2018. *
  https://arxiv.org/abs/1810.00115
- “**Numerical and Perturbative Computations of the Fuzzy Dark Matter Model**,” X. Li, L. Hui, G. Bryan, arXiv:1801.01915 [astro-ph.CO], October 3, 2018. *
  https://arxiv.org/abs/1810.01915
- “**The Impact of Radio AGN Bubble Composition On the Dynamics and Thermal Balance of the Intracluster Medium**,” H.-Y. Yang, et al., arXiv:1810.04173 [astro-ph.HE], October 9, 2018. *
  https://arxiv.org/abs/1810.04173
- “**Turbulence Structure in a Stratocumulus Cloud**,” G. Matheou, Atmosphere, vol.9, issue 10, October 10, 2018. *
  https://www.mdpi.com/2073-4433/9/10/392
- “**Dynamics of Multiple Protoplanets Embedded in Gas and Pebble Disks and its Dependence on Σ and ν Parameters**,” M. Broz, O. Chrenko, D. Nesvorny, M. Lambrechts, Astronomy & Astrophysics, October 14, 2018. *
  https://www.aanda.org/articles/aa/pdf/forth/aa33855-18.pdf

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

Papers (cont.)

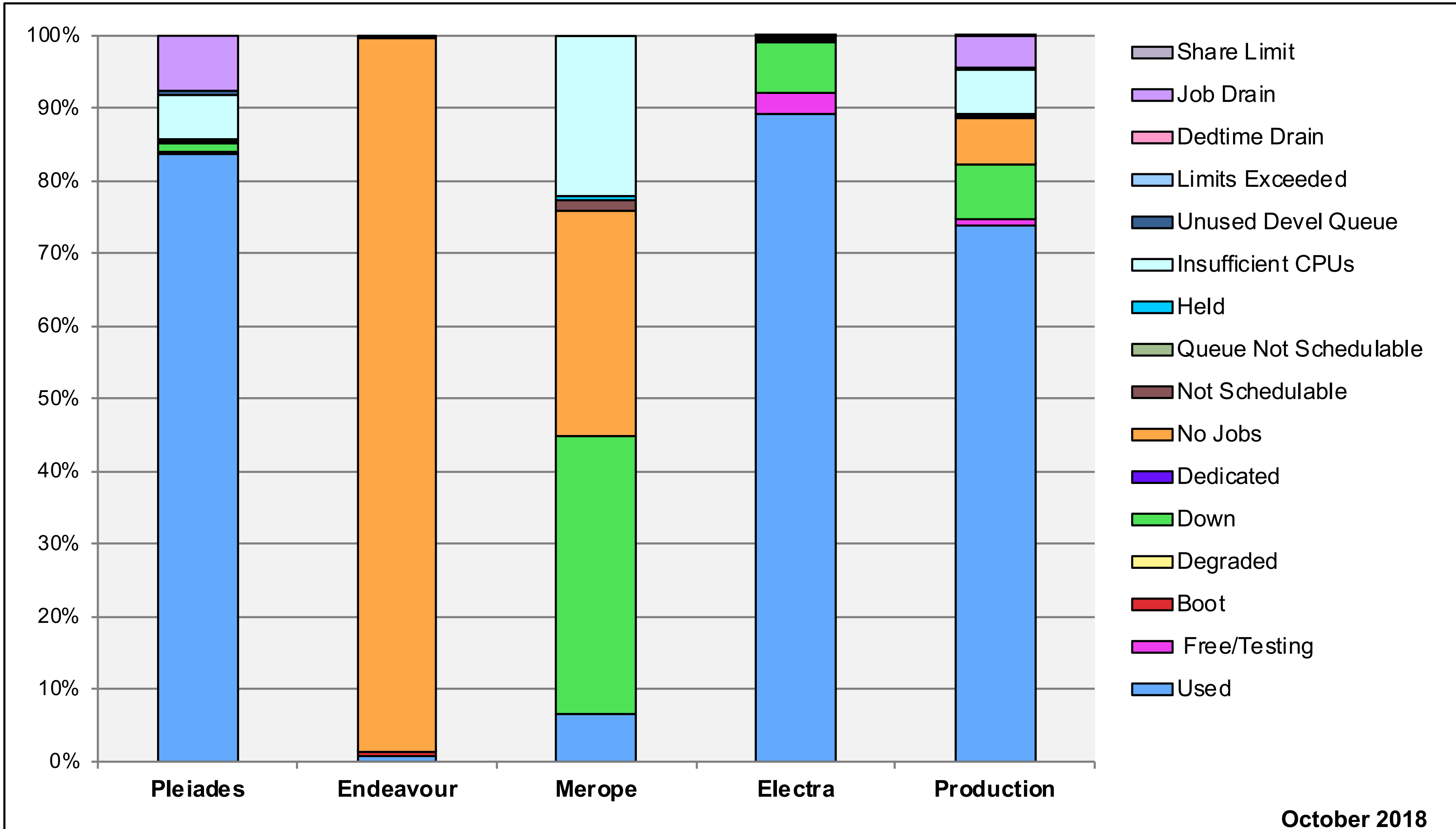
- "**Figuring Out Gas and Galaxies in Enzo (FOGGIE). I. Resolving Simulated Circumgalactic Absorption at 2<z<2.5**," M. Peeples, et al., arXiv:1810.06566 [astro-ph.GA], October 15, 2018. *
  https://arxiv.org/abs/1810.06566
- "**New Formation Models for the Kepler-36 System**," P. Bodenheimer, D. Stevenson, J. Lissauer, G. D'Angelo, arXiv:1808.07160 [astro-ph.EP], October 16, 2018. *
  https://arxiv.org/abs/1810.07160
- "**Hydrocode Simulations of Asteroid Airbursts and Constraints for Tunguska**," D. Robertson, D. Mathias, Icarus, published online October 21, 2018. *
  https://www.sciencedirect.com/science/article/pii/S0019103518304202
- "**O2 Solubility in Martian Near-Surface Environments and Implications for Aerobic Life**," V. Stamenkovic, L. Ward, M. Mischna, W. Fischer, Nature Geoscience, October 22, 2018. *
  https://www.nature.com/articles/s41561-018-0243-0
- "**Relativistic-Electron-Driven Magnetic Reconnection in the Laboratory**," A. E. Raymond, et al., Physical Review E, vol. 98, October 24, 2018. *
  https://journals.aps.org/pre/abstract/10.1103/PhysRevE.98.043207
- "**Partitioning Ocean Motions into Balanced Motions and Internal Gravity Waves: A Modeling Study in Anticipation of Future Space Missions**," H. Torres, et al., Journal of Geophysical Research: Oceans, October 26, 2018. *
  https://agupubs.onlinelibrary.wiley.com/doi/abs/10.1029/2018JC014438

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

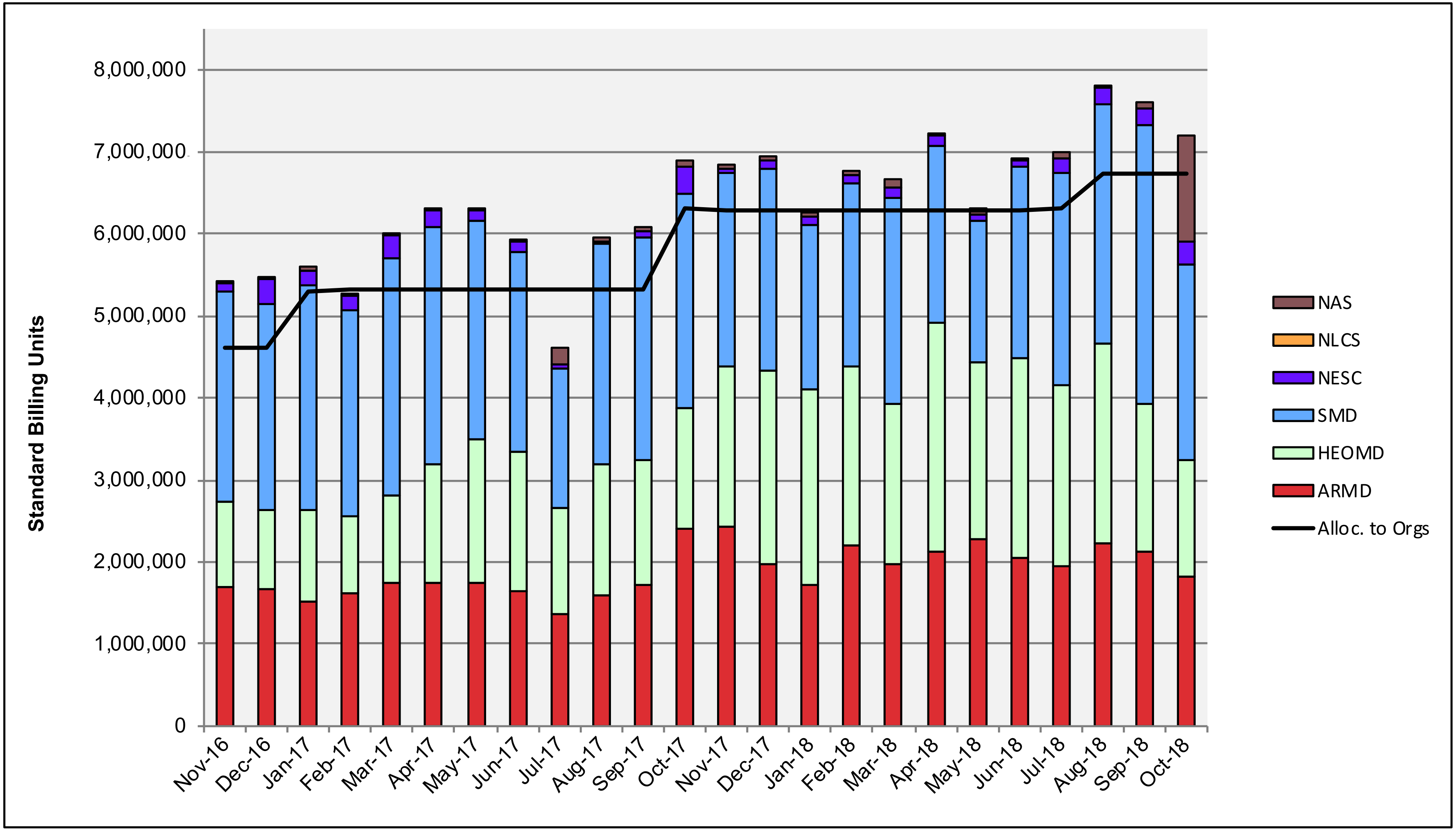
News and Events

- **Is There a Giant Plant Lurking Beyond Pluto?** *IEEE Spectrum*, October 3, 2018—A race is on to discover Planet Nine using classical astronomy and new computational techniques, including work by researchers at the Southwest Research Institute in Colorado, who are using the Pleiades supercomputer to run detailed models of the formation of the Kuiper Belt and discover what happens when they add a planet into the mix. *https://spectrum.ieee.org/aerospace/satellites/is-there-a-giant-planet-lurking-beyond-pluto*
- **'Pulsar in a Box' Reveals Surprising Picture of a Neutron Star's Surroundings**, *NASA Press Release*, October 10, 2018—A simulation run on NASA's Pleiades and Discover supercomputers yields a more detailed understanding of the complex, high-energy environment around spinning neutron stars called pulsars. *https://www.nasa.gov/feature/goddard/2018/pulsar-in-a-box-reveals-surprising-picture-of-a-neutron-star-s-surroundings*
  - **Hidden Secrets of Pulsars Revealed by Trippy Computer Simulations**, *Gizmodo*, October 10, 2018. *https://gizmodo.com/hidden-secrets-of-pulsars-revealed-by-trippy-computer-s-1829662417*
- **Video: Supercomputing the Secrets of Giant Stars**, *insideHPC*, October 21, 2018—In this video, supercomputing power and algorithms help astrophysicists untangle giant stars' brightness, temperature, and chemical variations. Researchers used the Pleiades supercomputer to perform some of their simulations. *https://insidehpc.com/2018/10/video-supercomputing-secrets-giant-stars/*

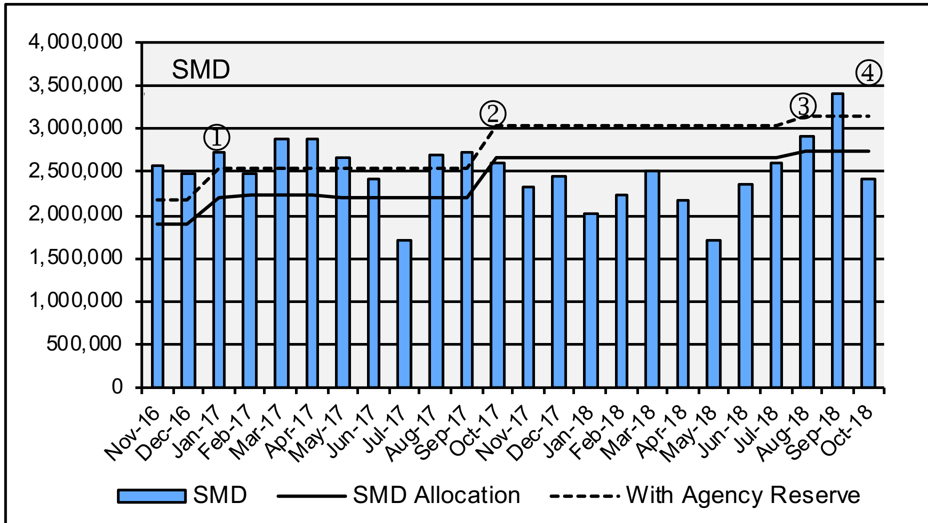
HECC Utilization

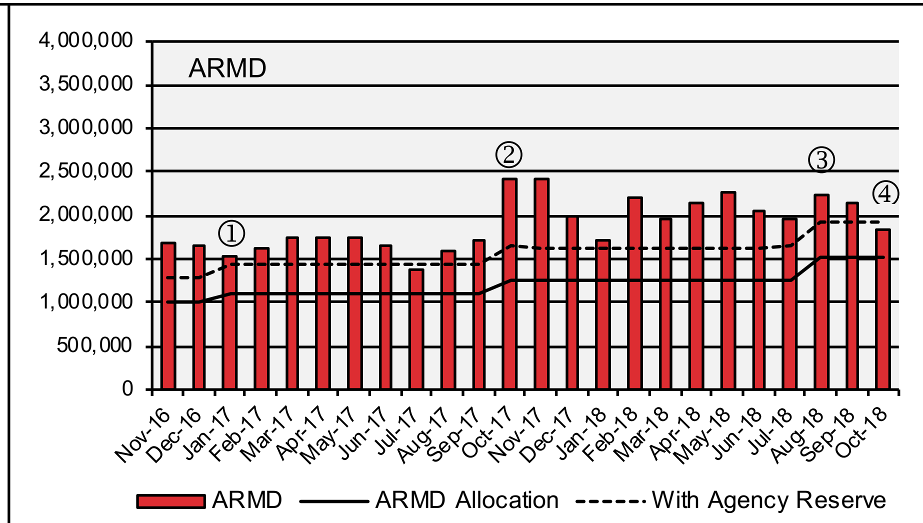


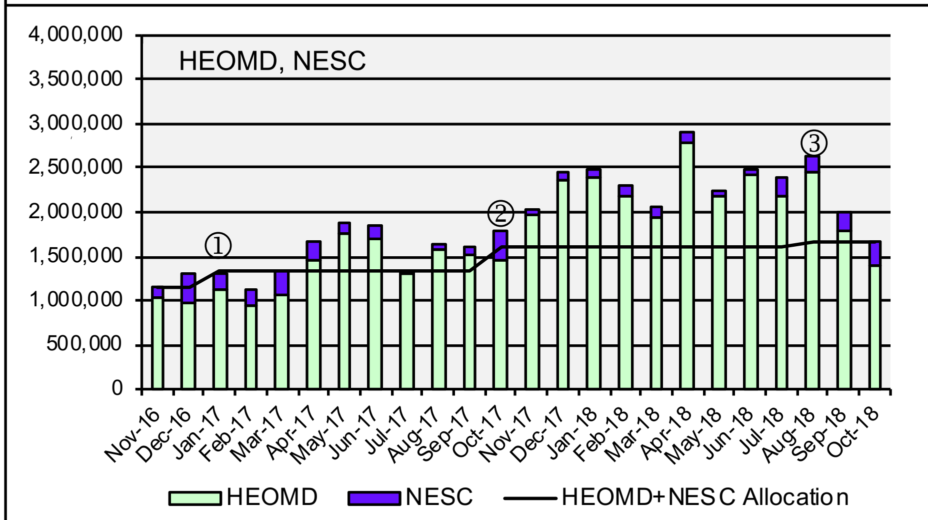
HECC Utilization Normalized to 30-Day Month



HECC Utilization Normalized to 30-Day Month







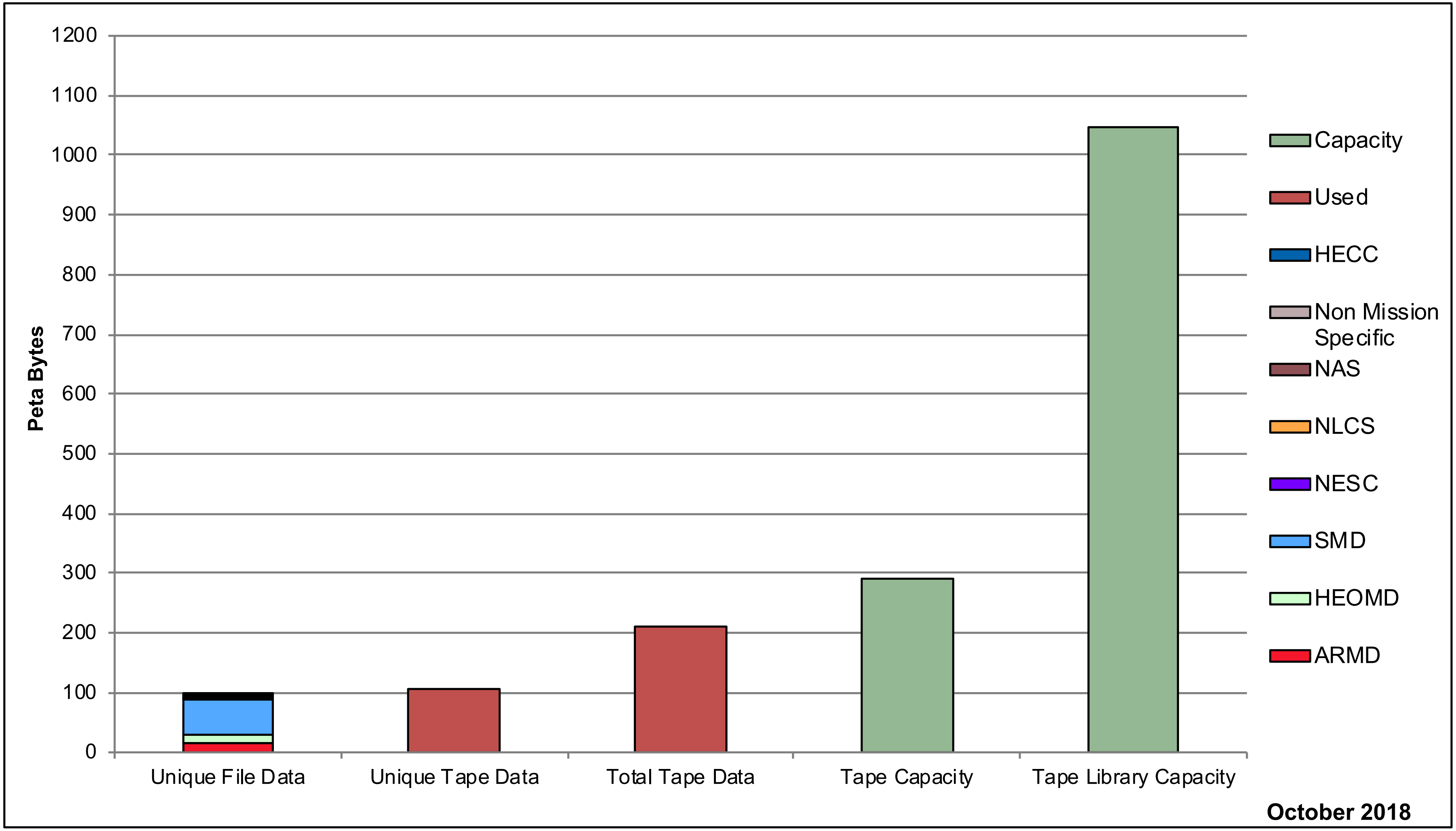
① 16 Broadwell racks added to Electra, 20 Westmere half racks added to Merope

② 4 Skylake E cells (16 D Rack Equivalence) added to Electra

③ 2 Skylake E cells (8 D Rack Equivalence) added to Electra; 1 rack is dedicated to ARMD

④ 2 Skylake E cells (8 D Rack Equivalence) added to Electra; 1 rack is dedicated to SMD

Tape Archive Status



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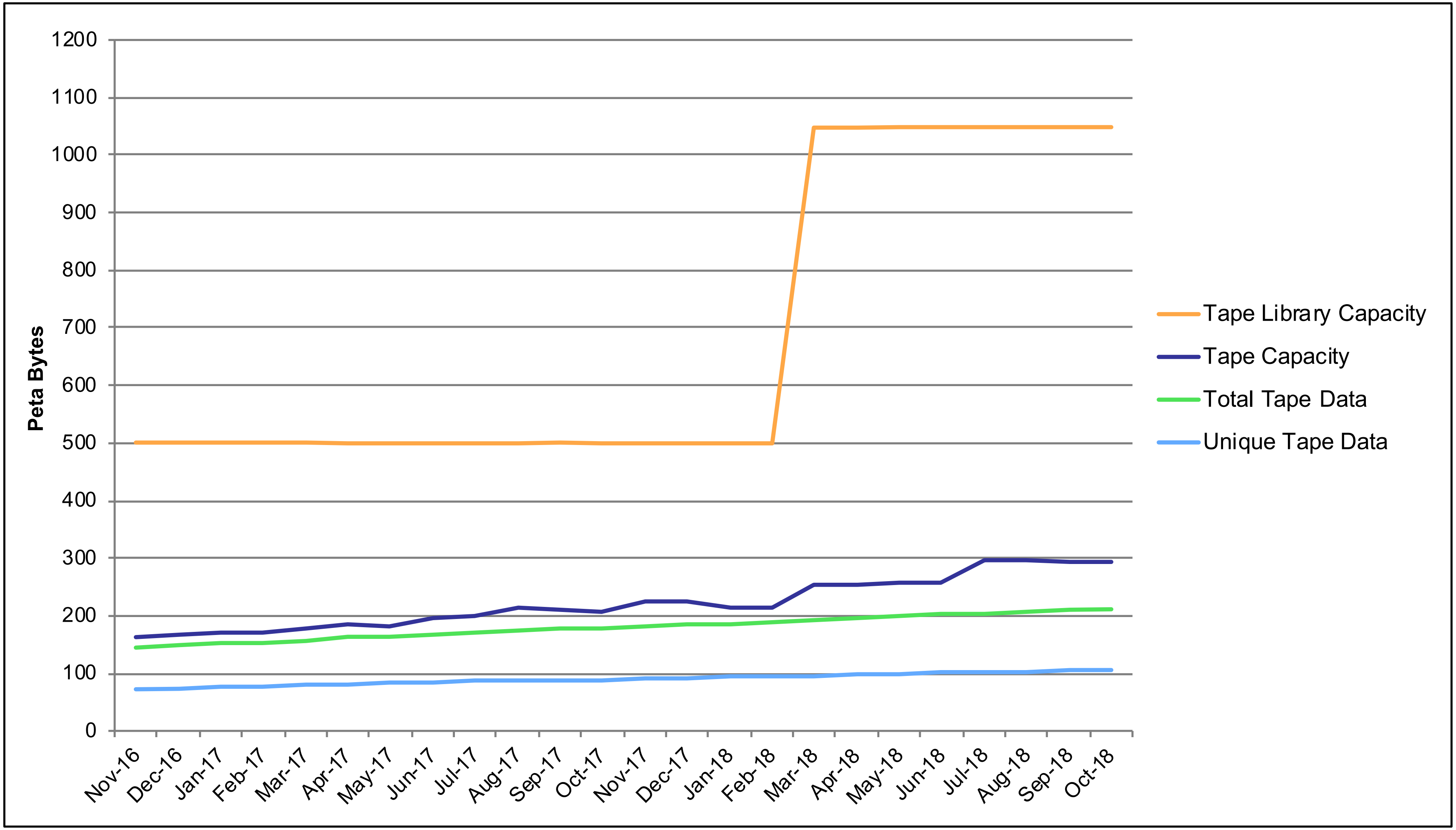
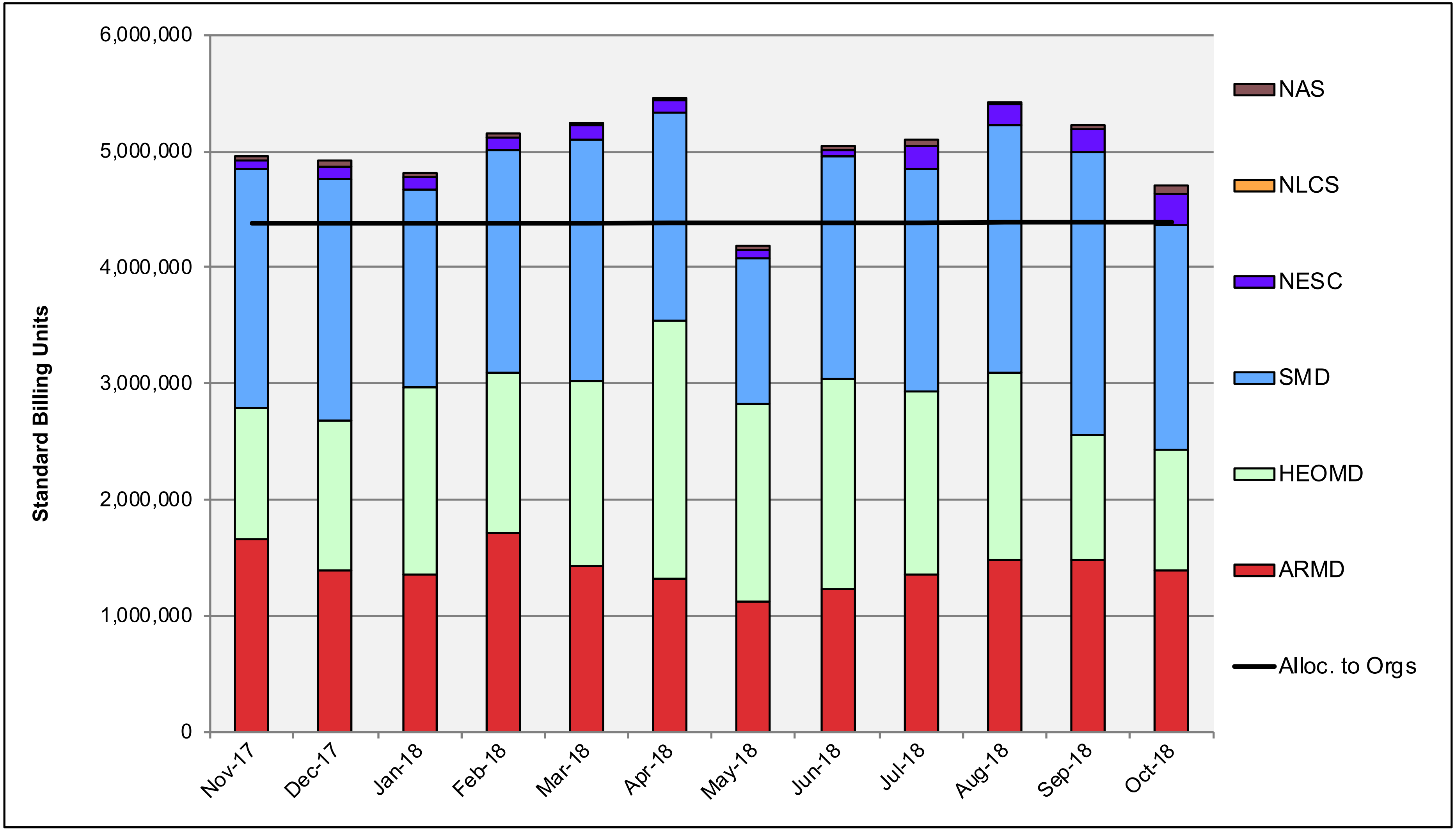
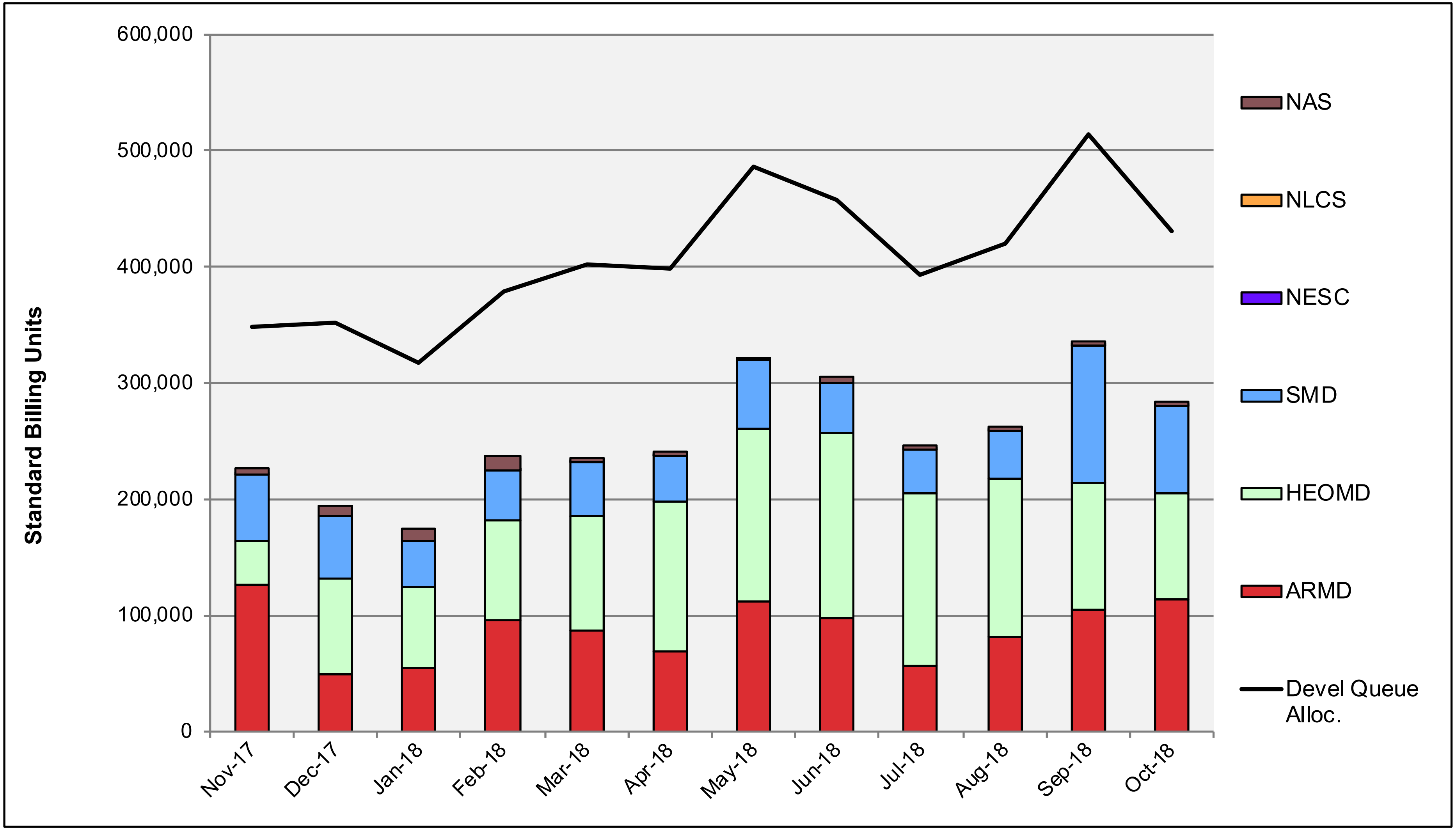


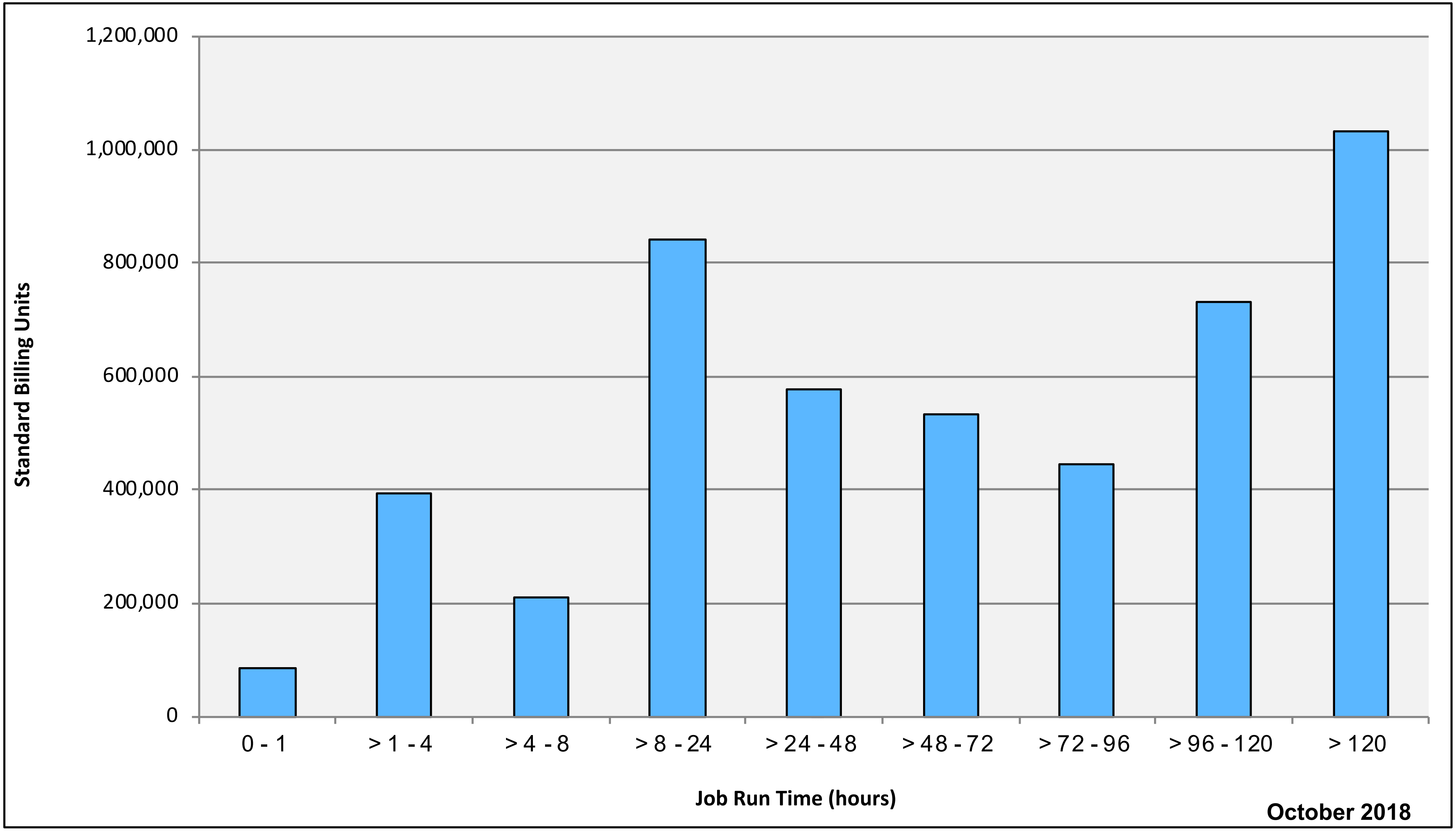
Pleiades: SBUs Reported, Normalized to 30-Day Month



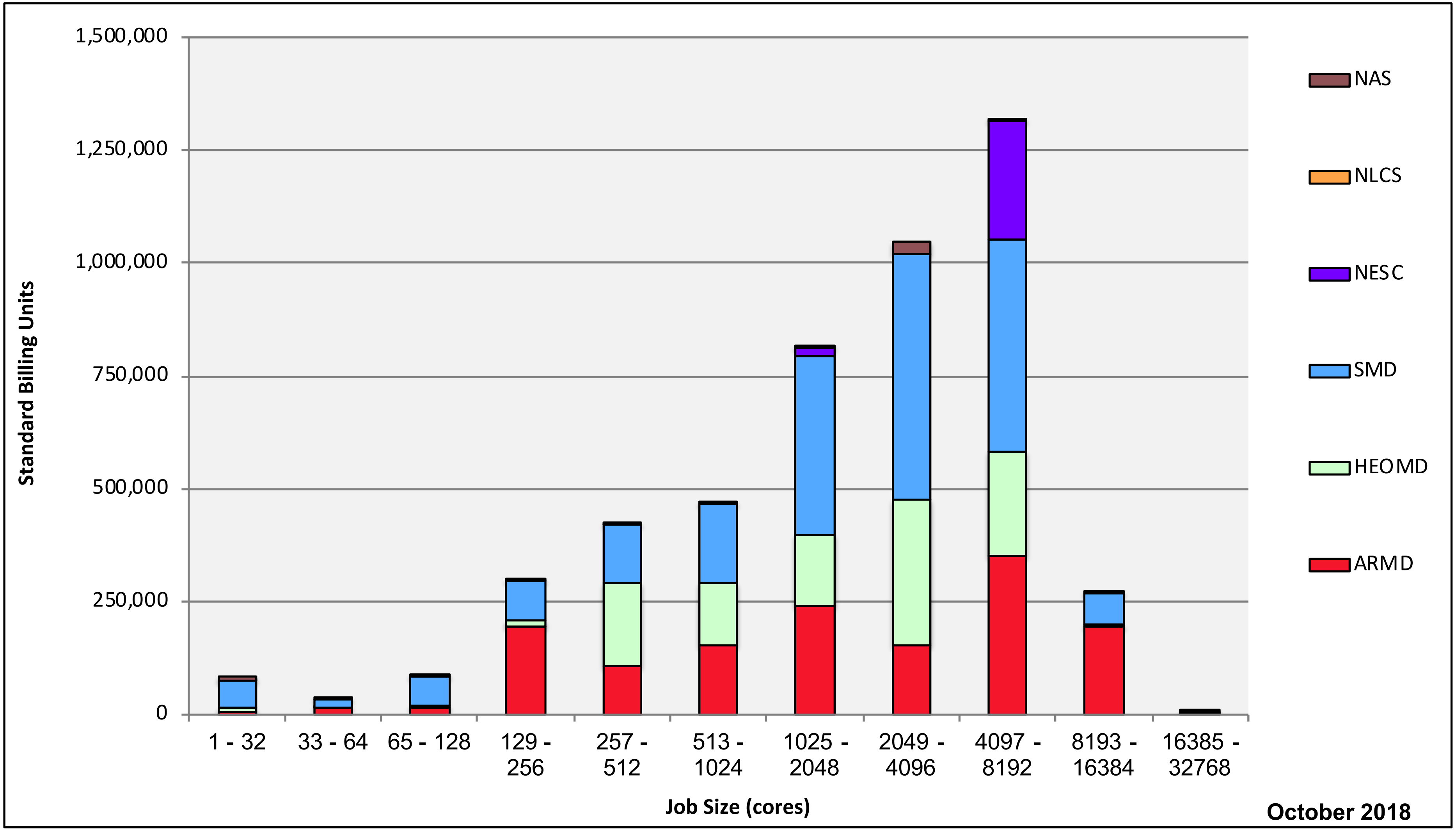
Pleiades:
Devel Queue Utilization



Pleiades: Monthly Utilization by Job Length



Pleiades:
Monthly Utilization by Size and Mission



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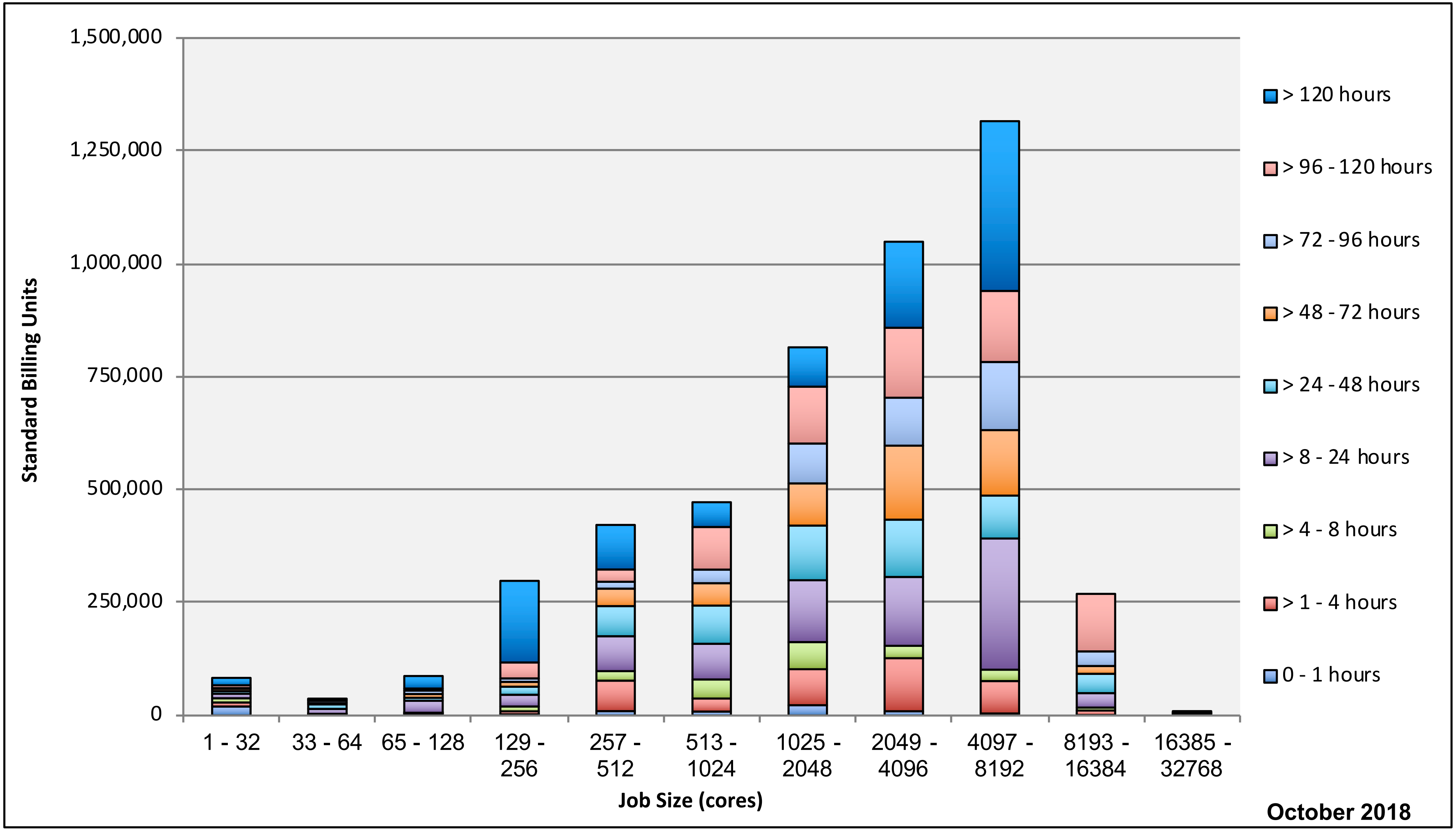
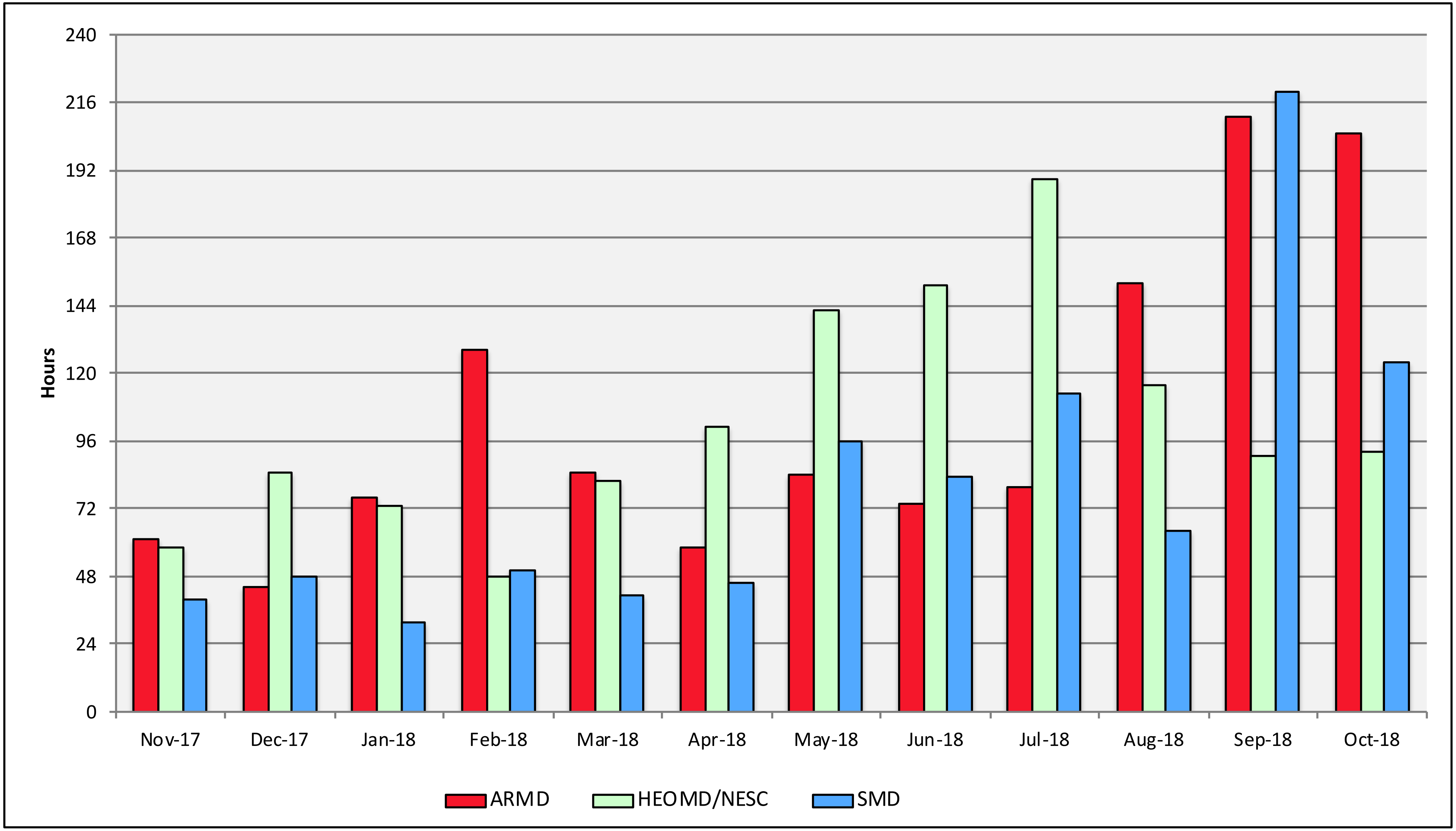
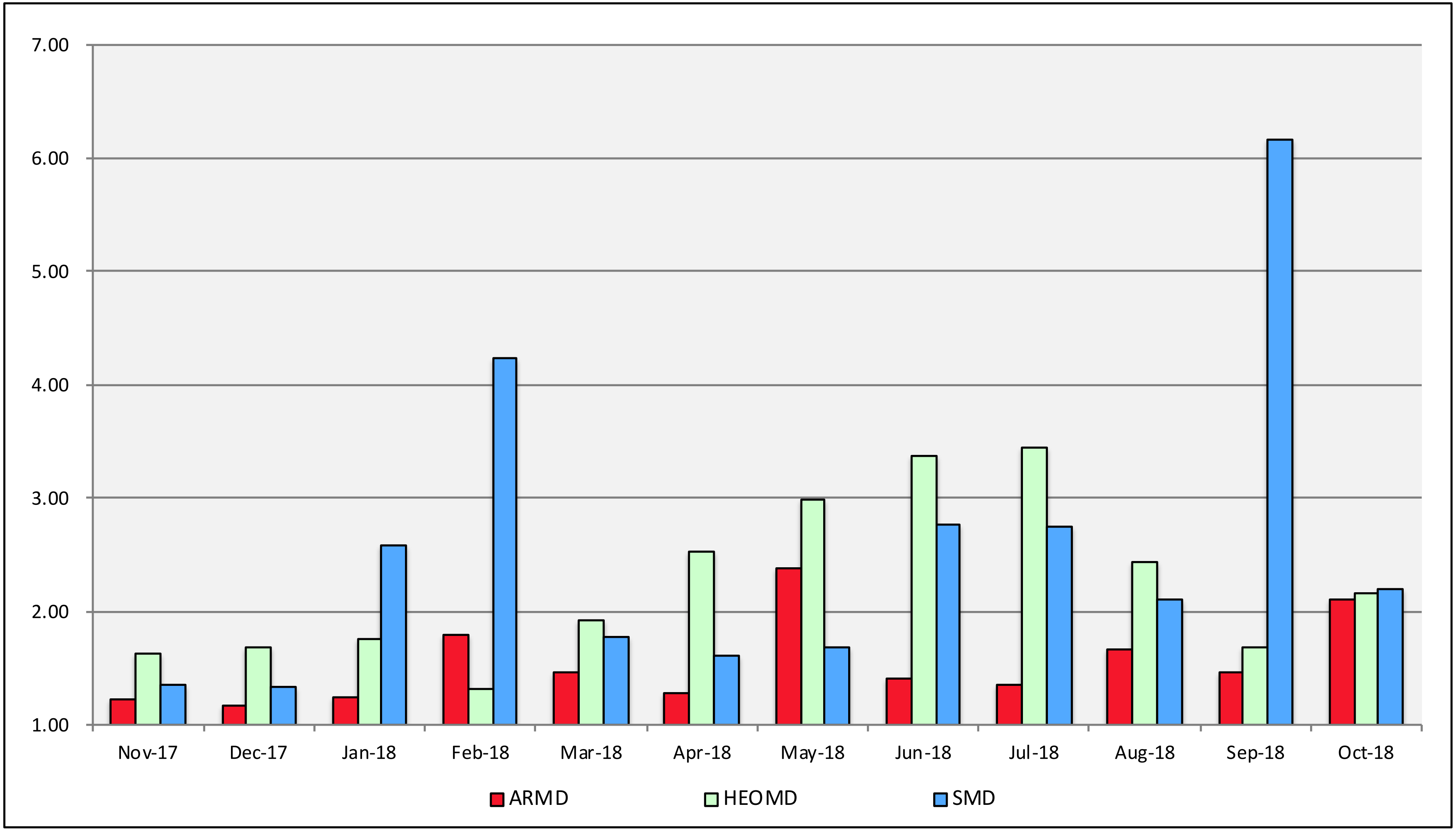


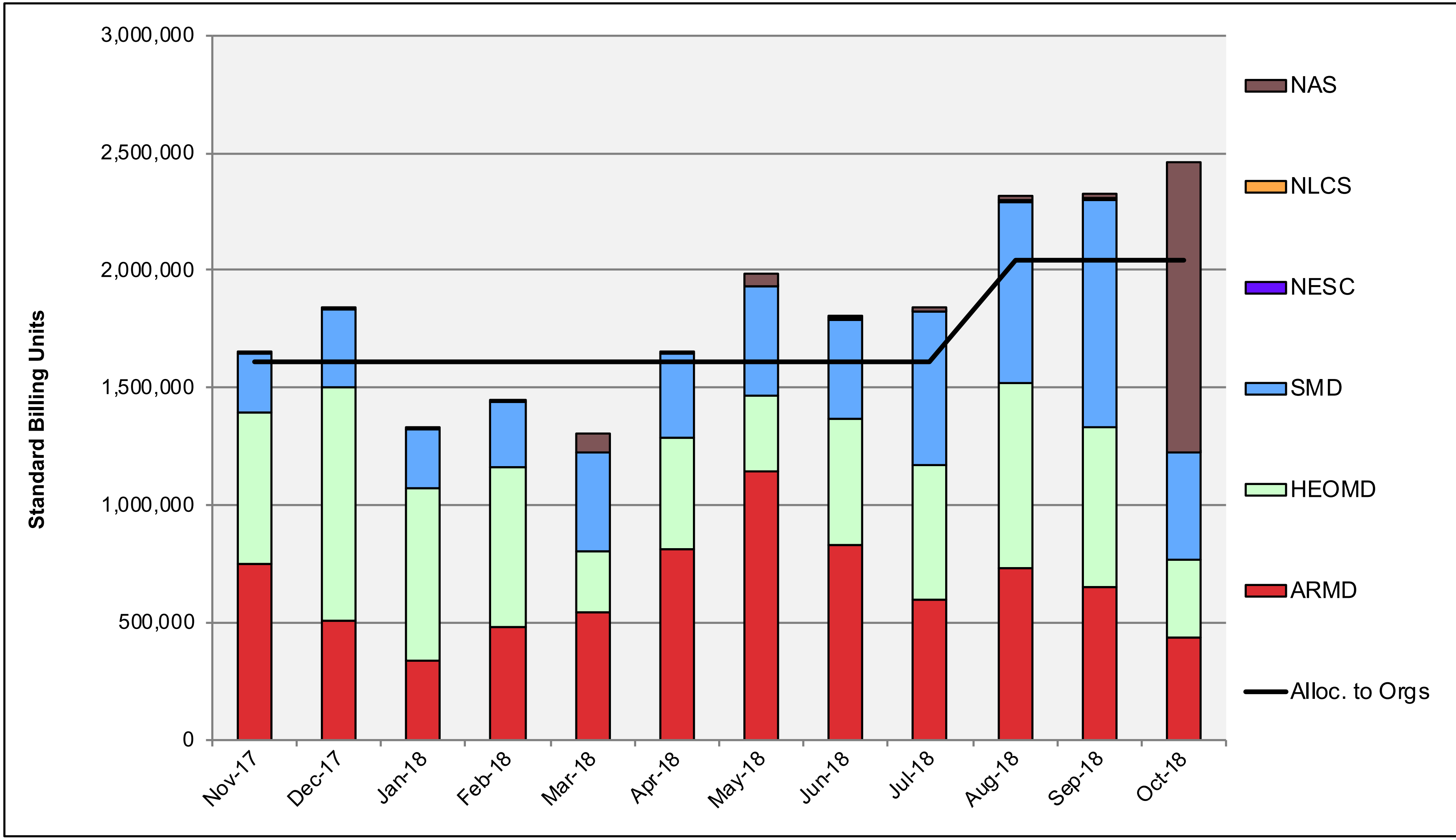
Pleiades: Average Time to Clear All Jobs



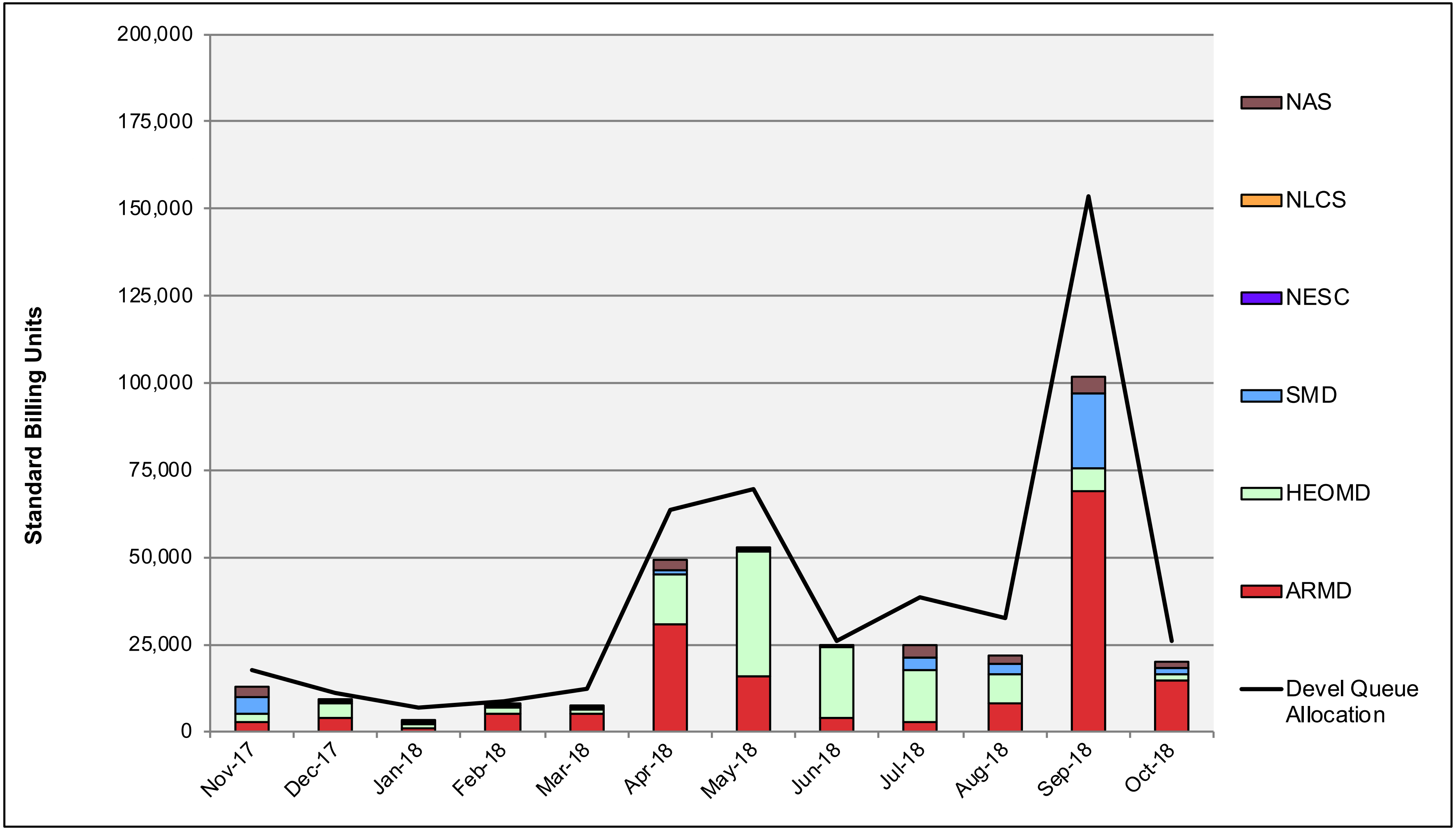
Pleiades: Average Expansion Factor



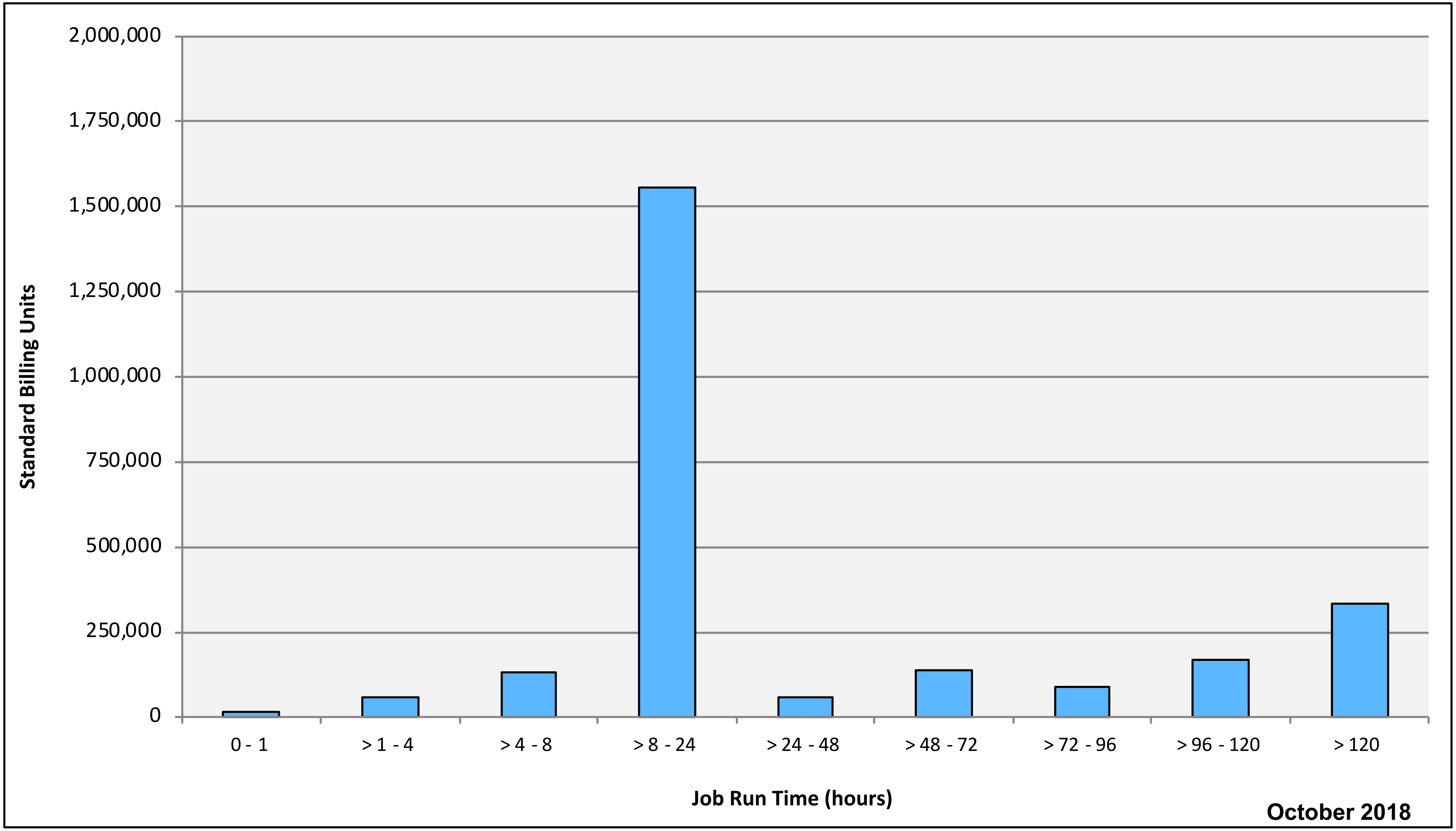
Electra:
SBUs Reported, Normalized to 30-Day Month



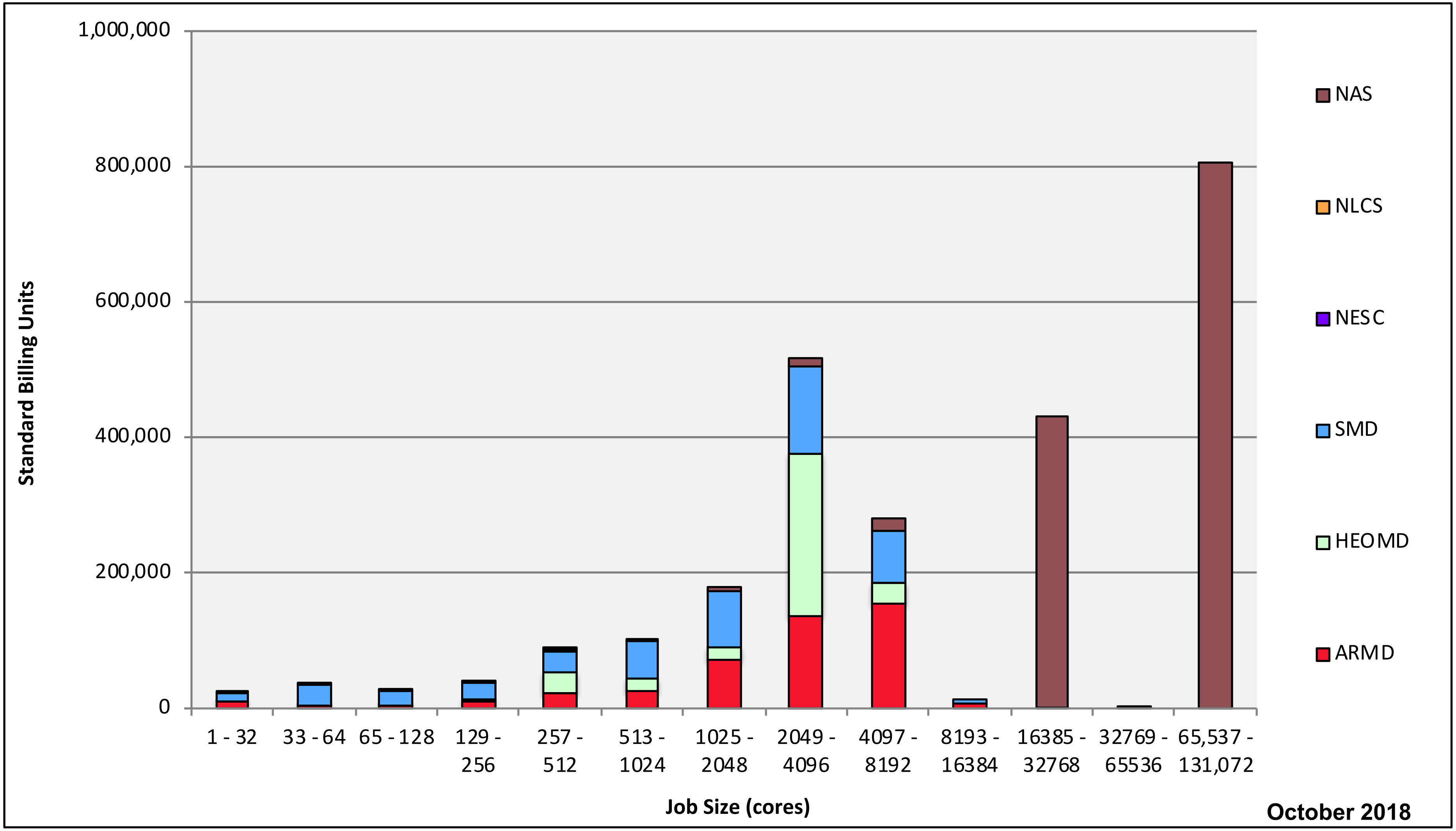
Electra: Devel Queue Utilization



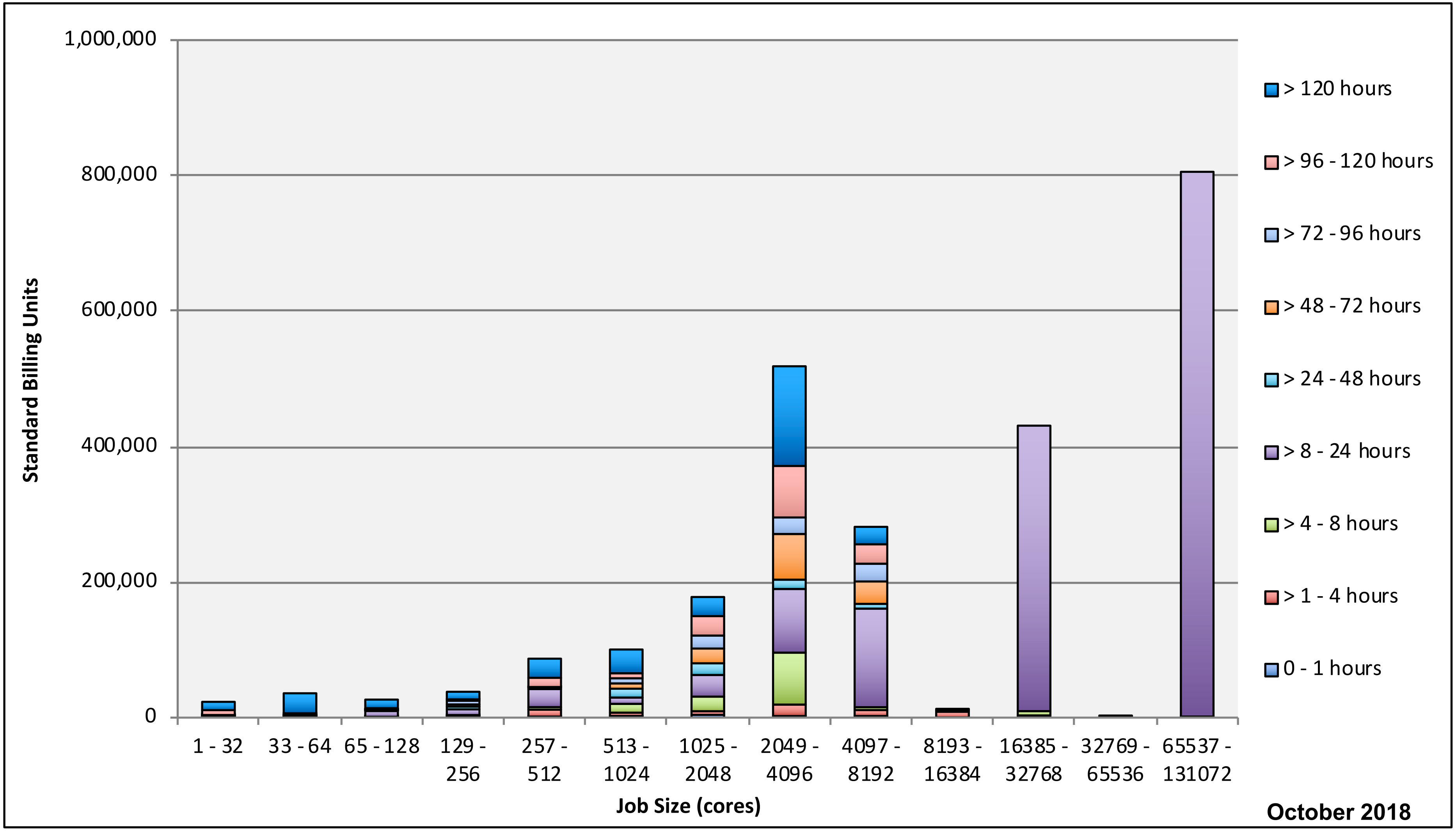
Electra: Monthly Utilization by Job Length



Electra: Monthly Utilization by Size and Mission



Electra:
Monthly Utilization by Size and Length



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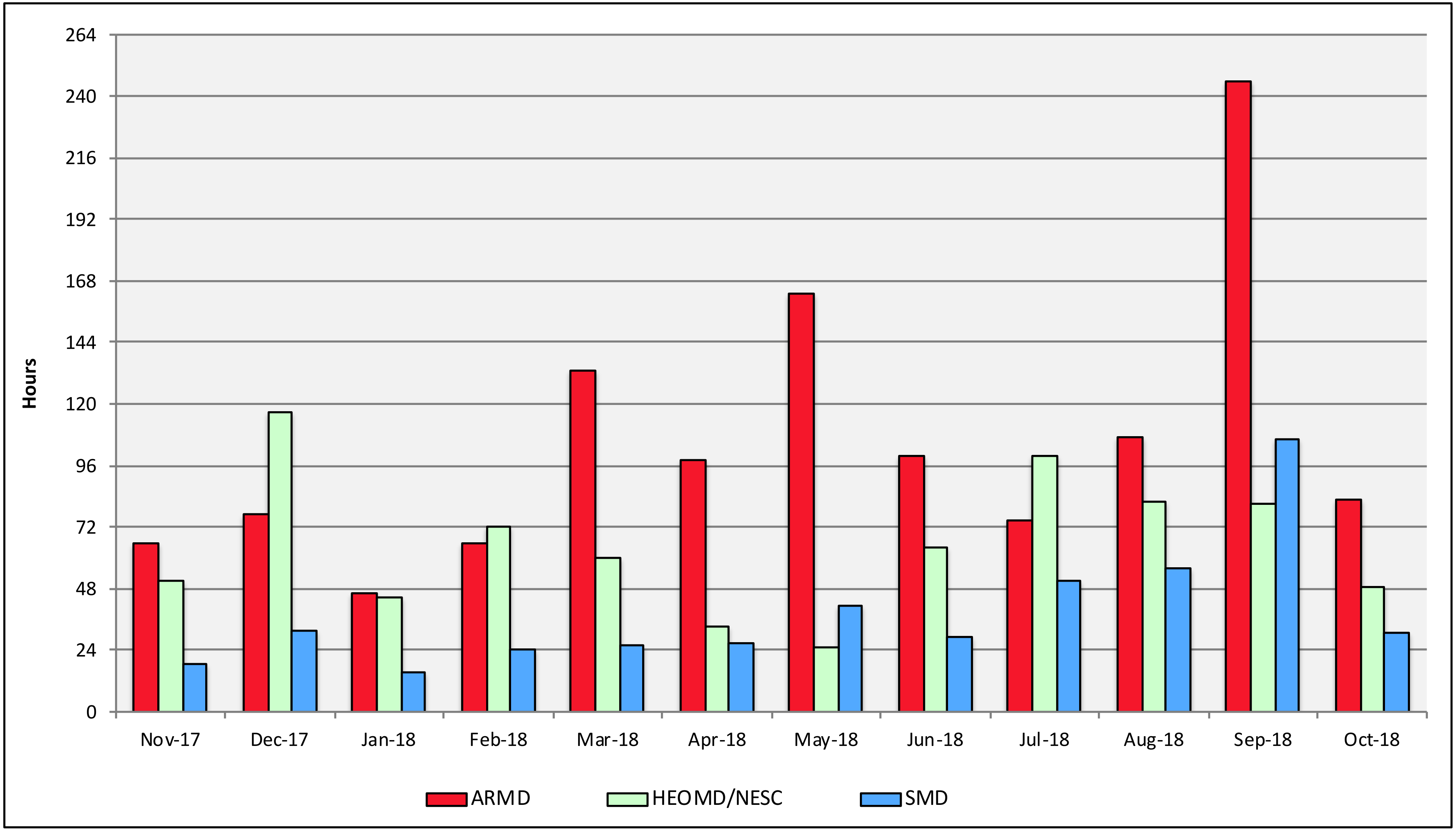
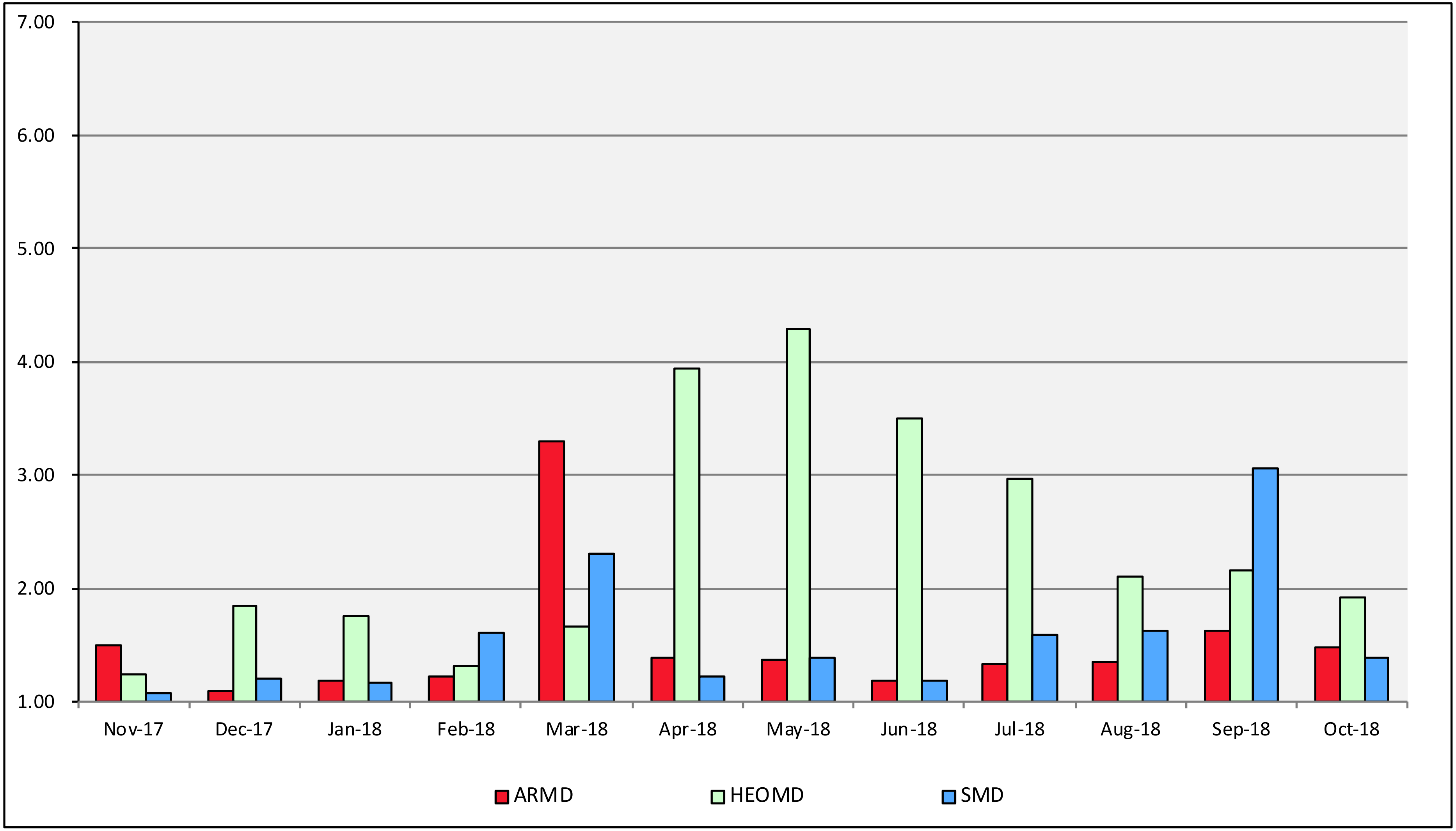
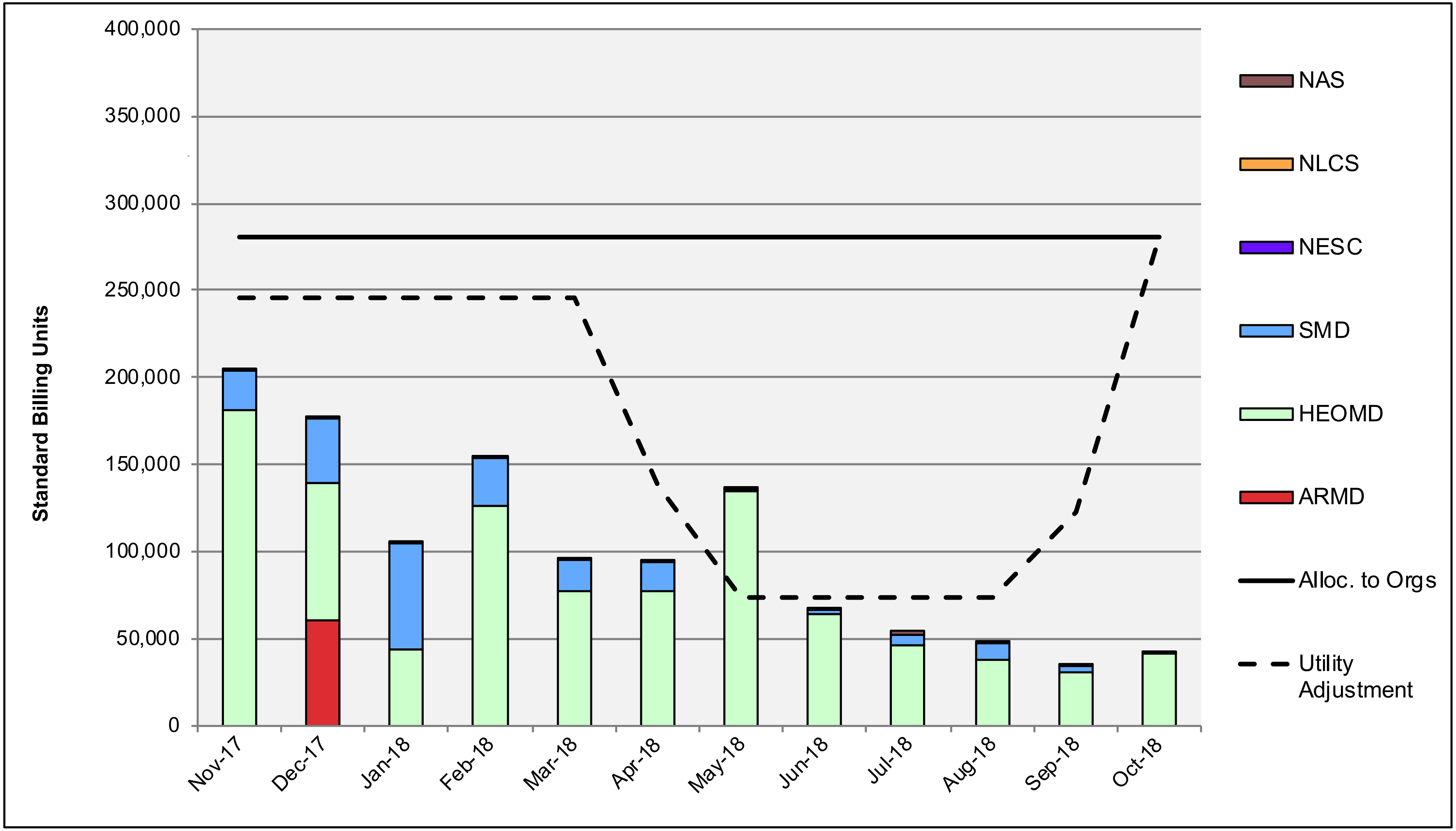


Electra:
Average Expansion Factor

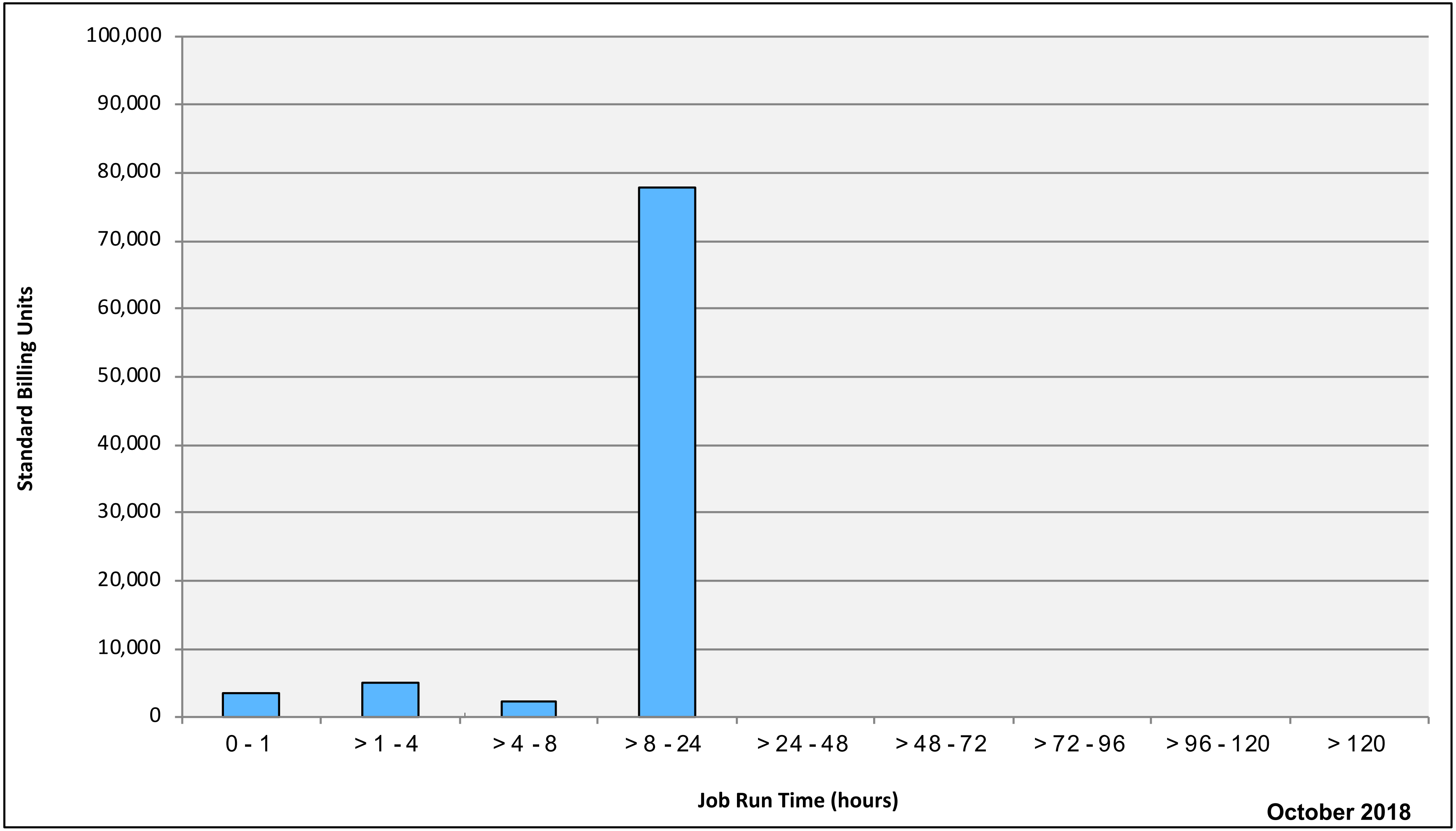


Merope: SBUs Reported, Normalized to 30-Day Month

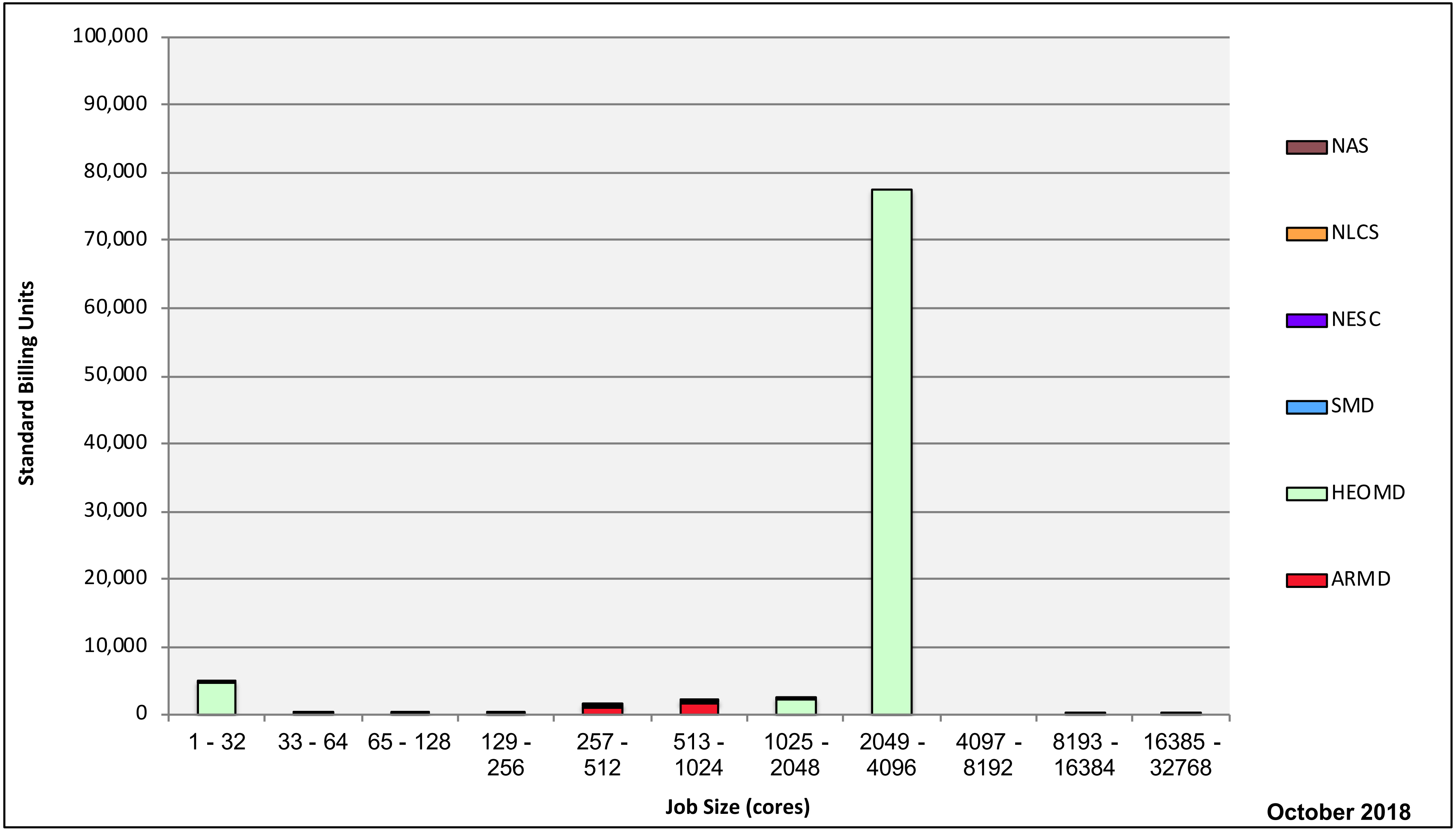


*Utility Adjustment: Multiple failures of chillers in N233A necessitated turning off a large portion of Merope

Merope:
Monthly Utilization by Job Length



Merope:
Monthly Utilization by Size and Mission



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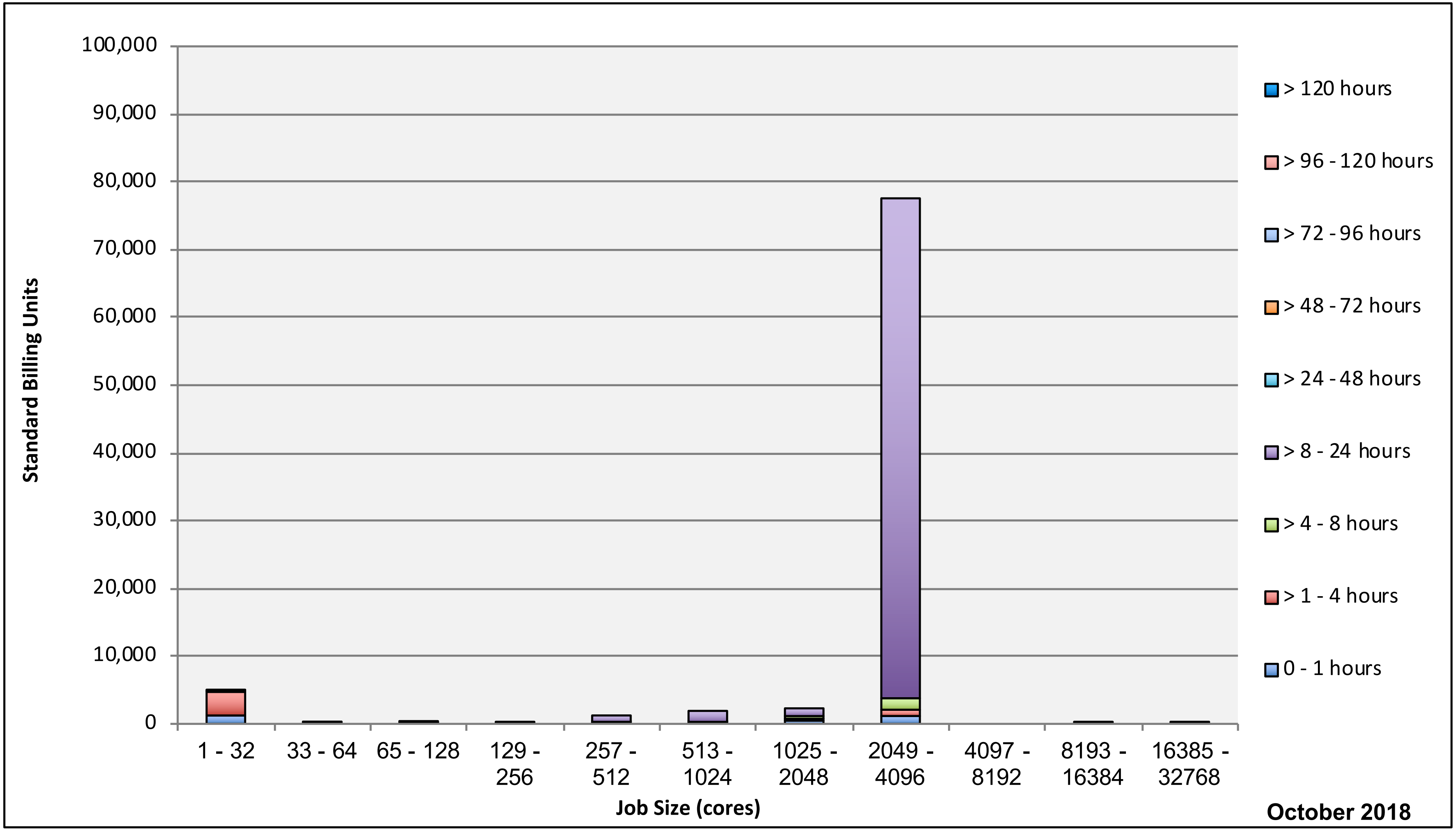

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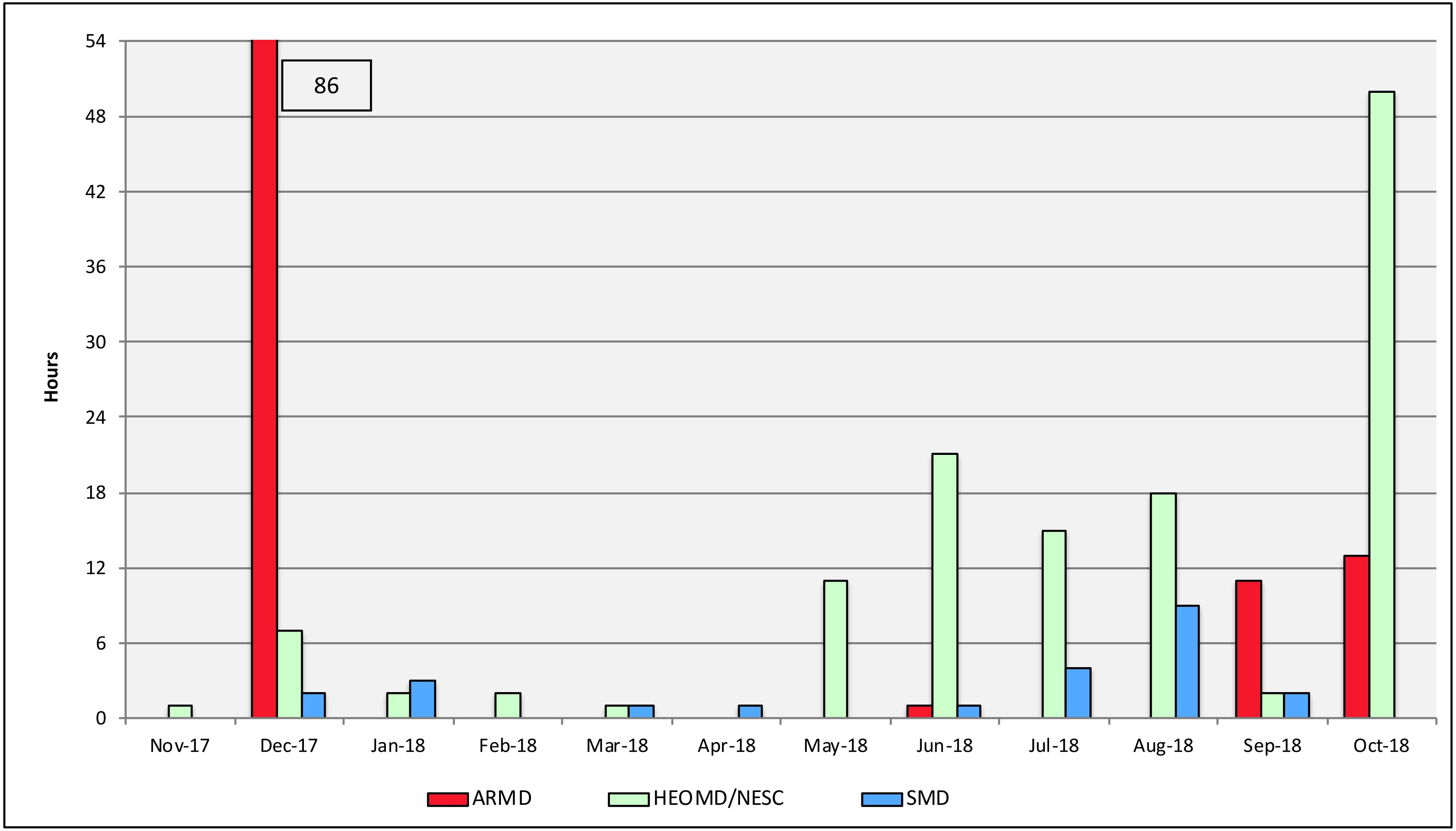
Average Time to Clear All Jobs



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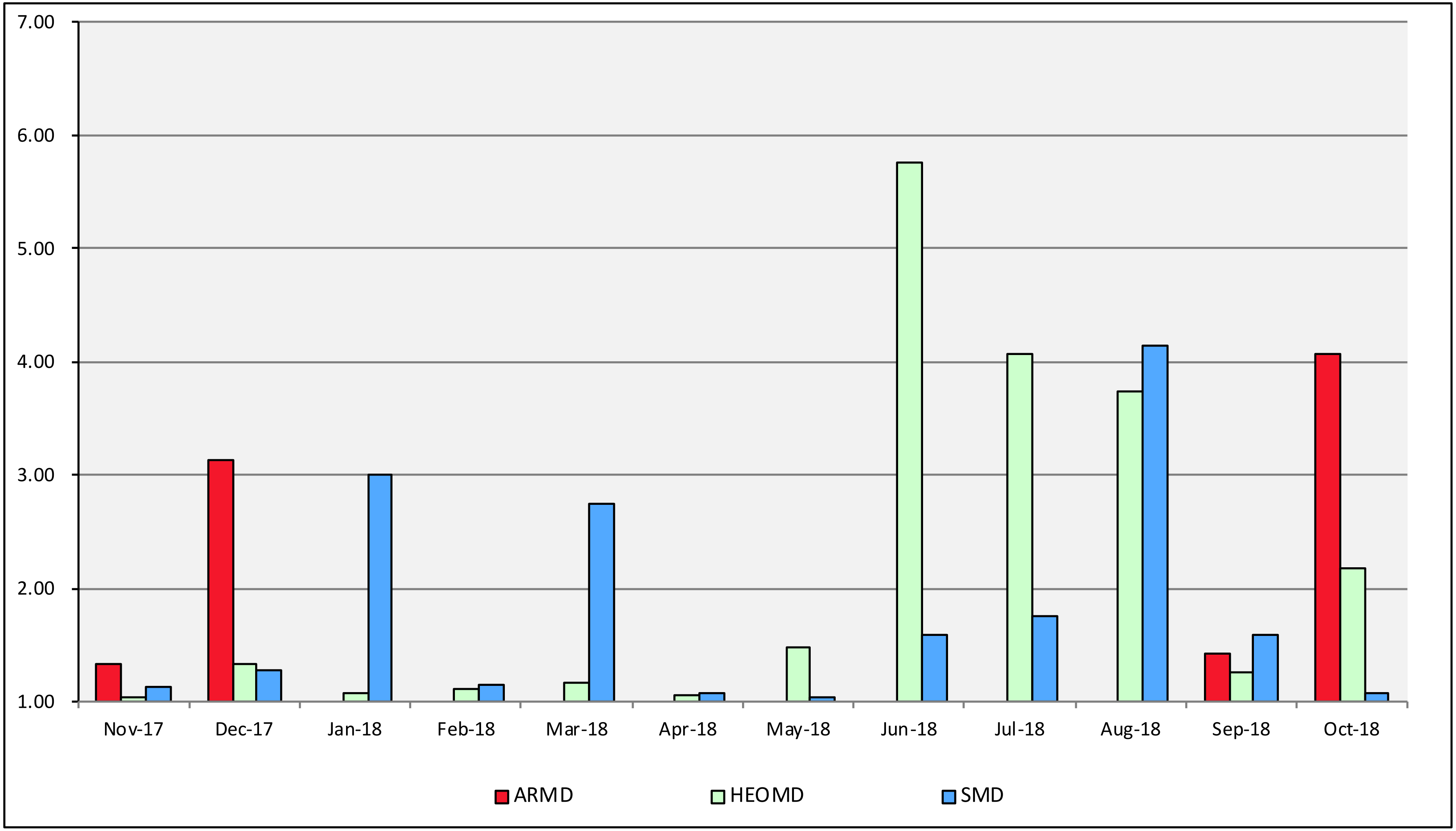
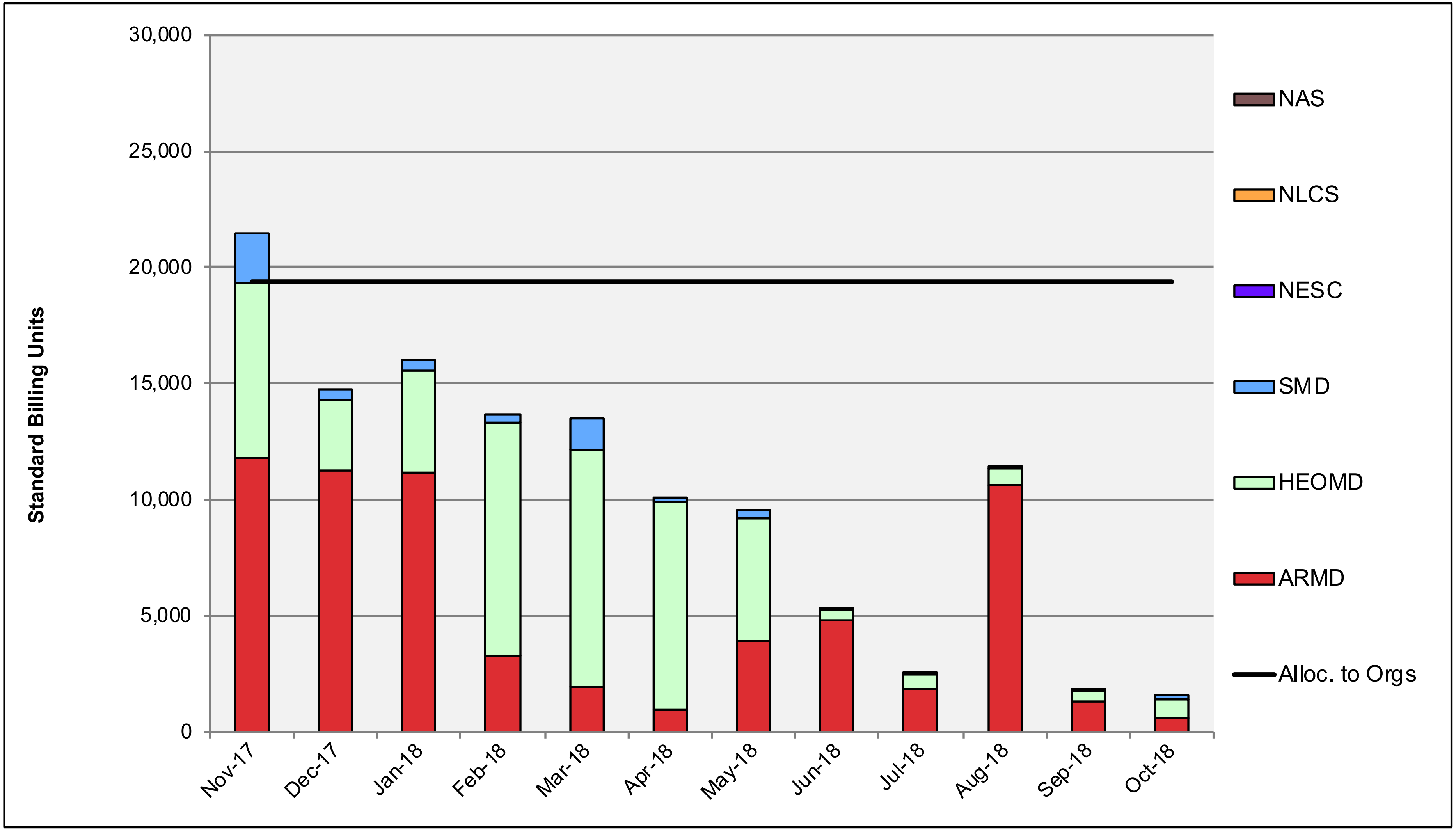
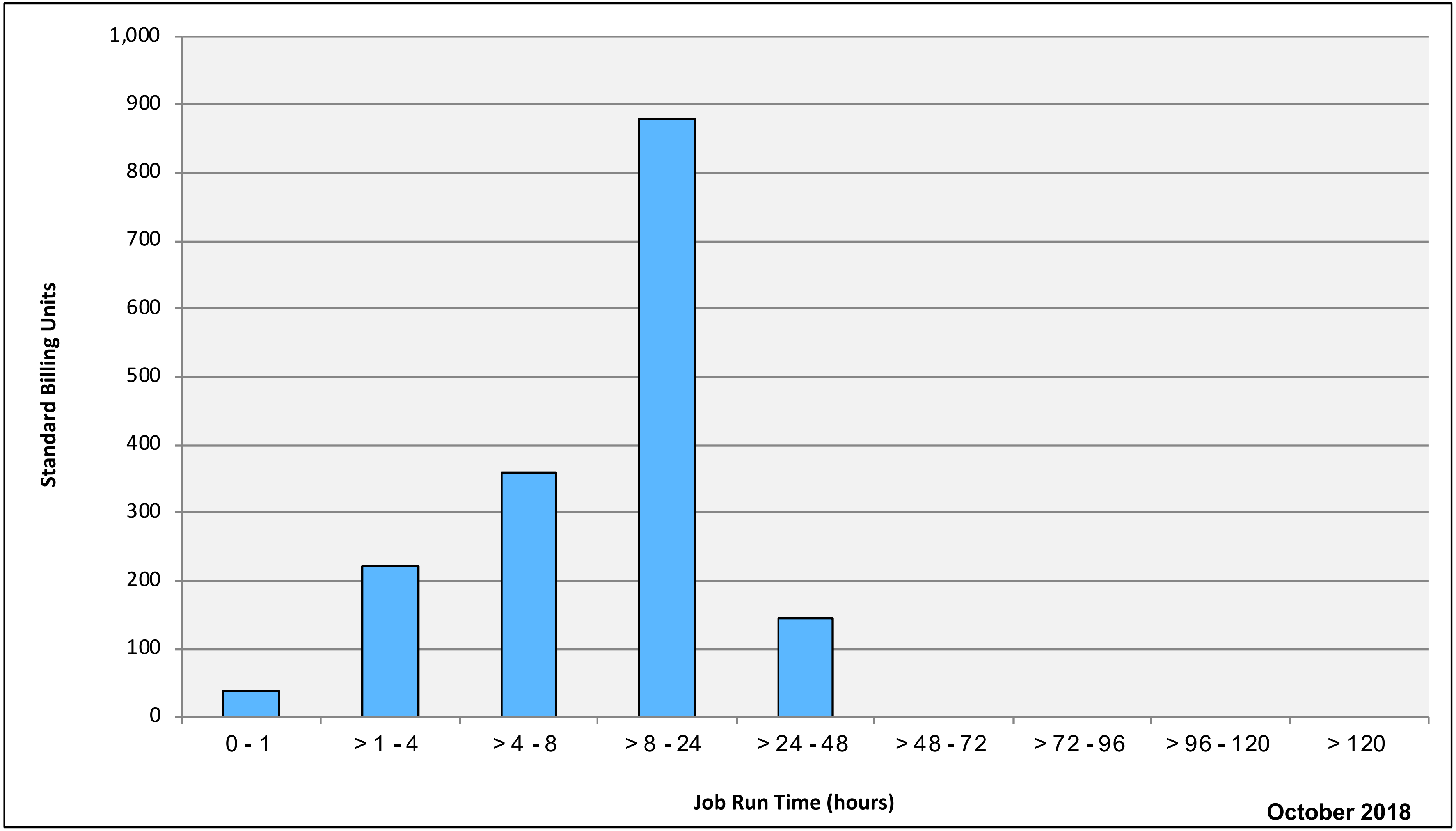


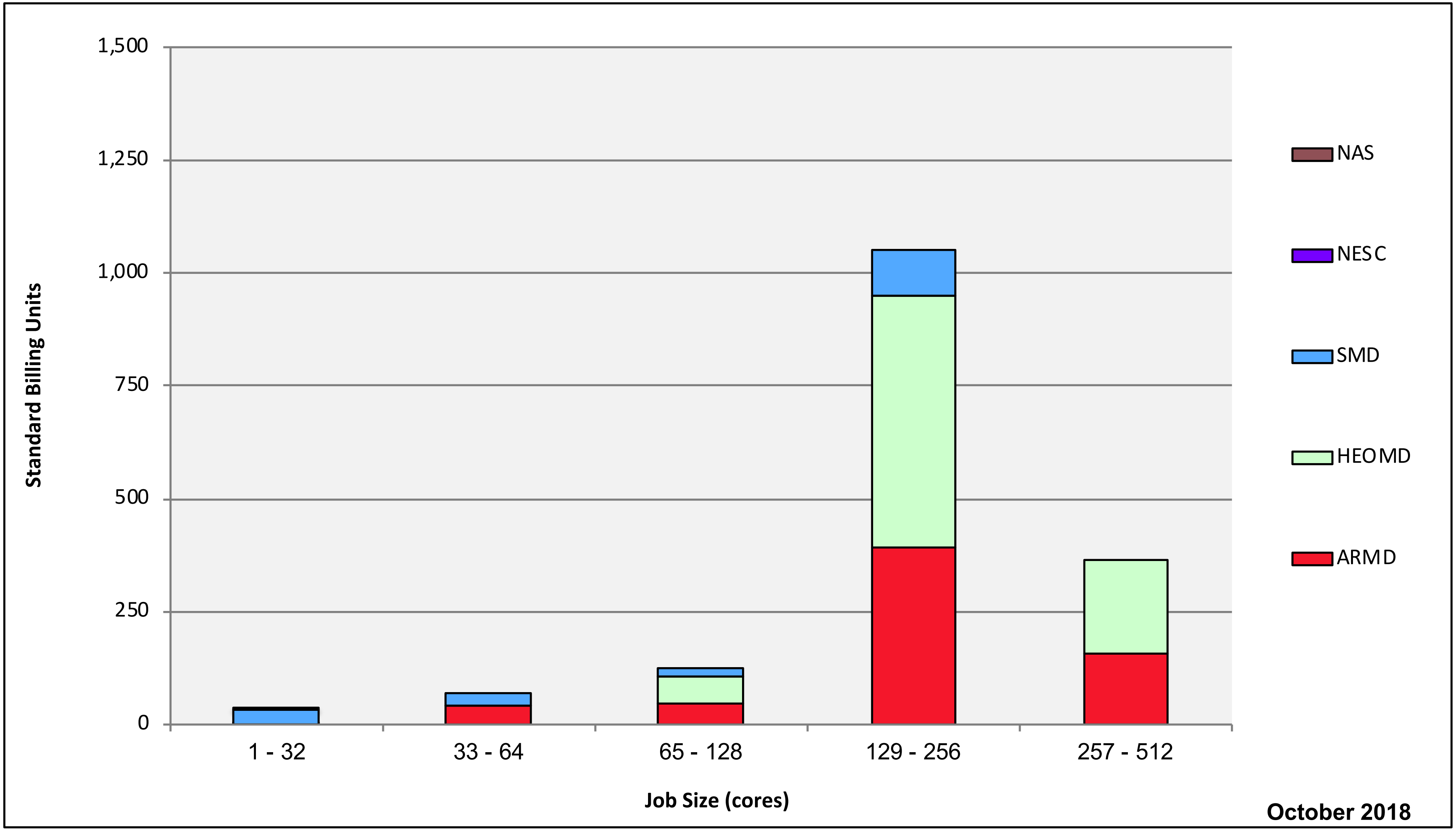
Endeavour: SBUs Reported, Normalized to 30-Day Month



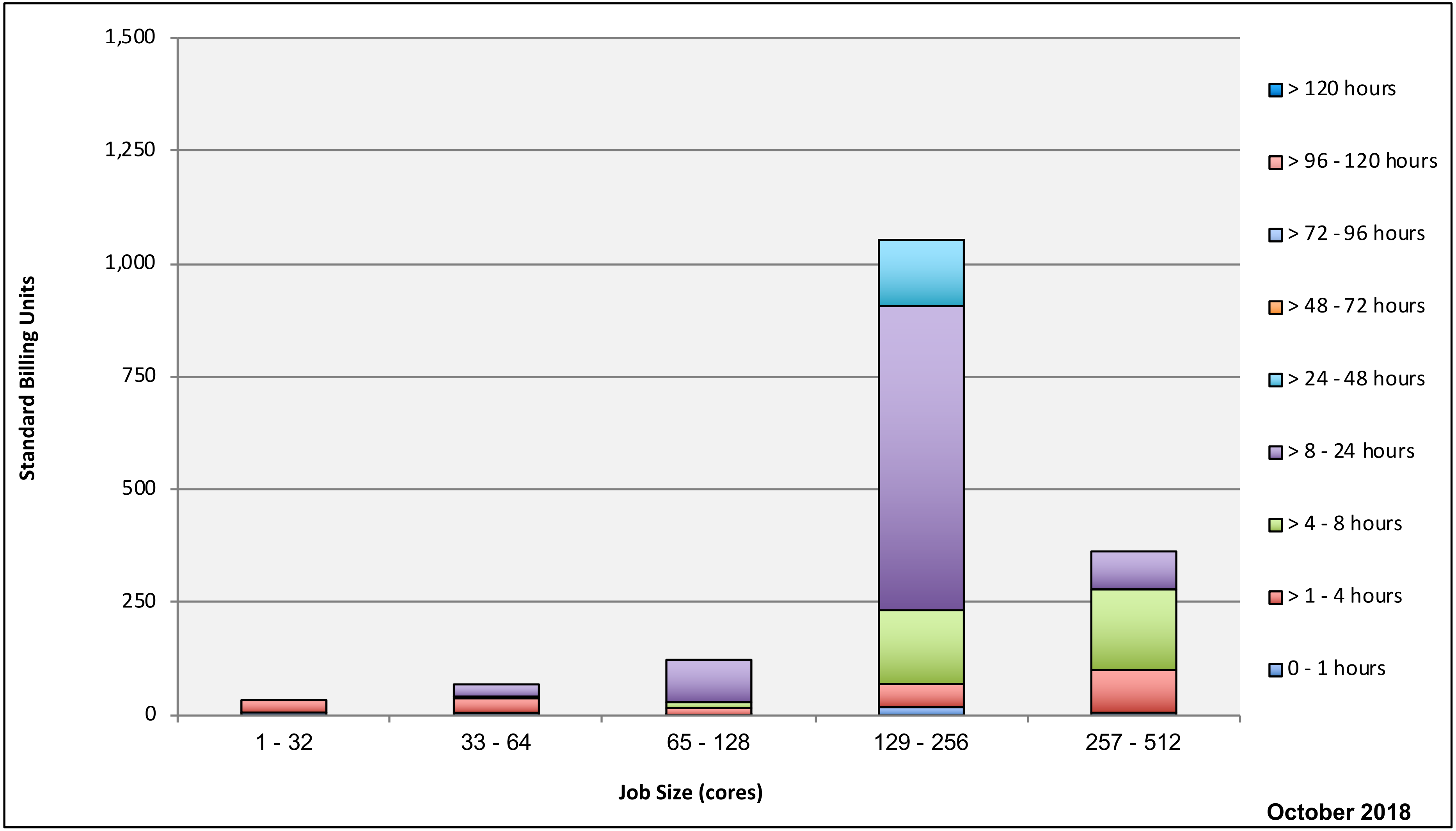
Endeavour:
Monthly Utilization by Job Length



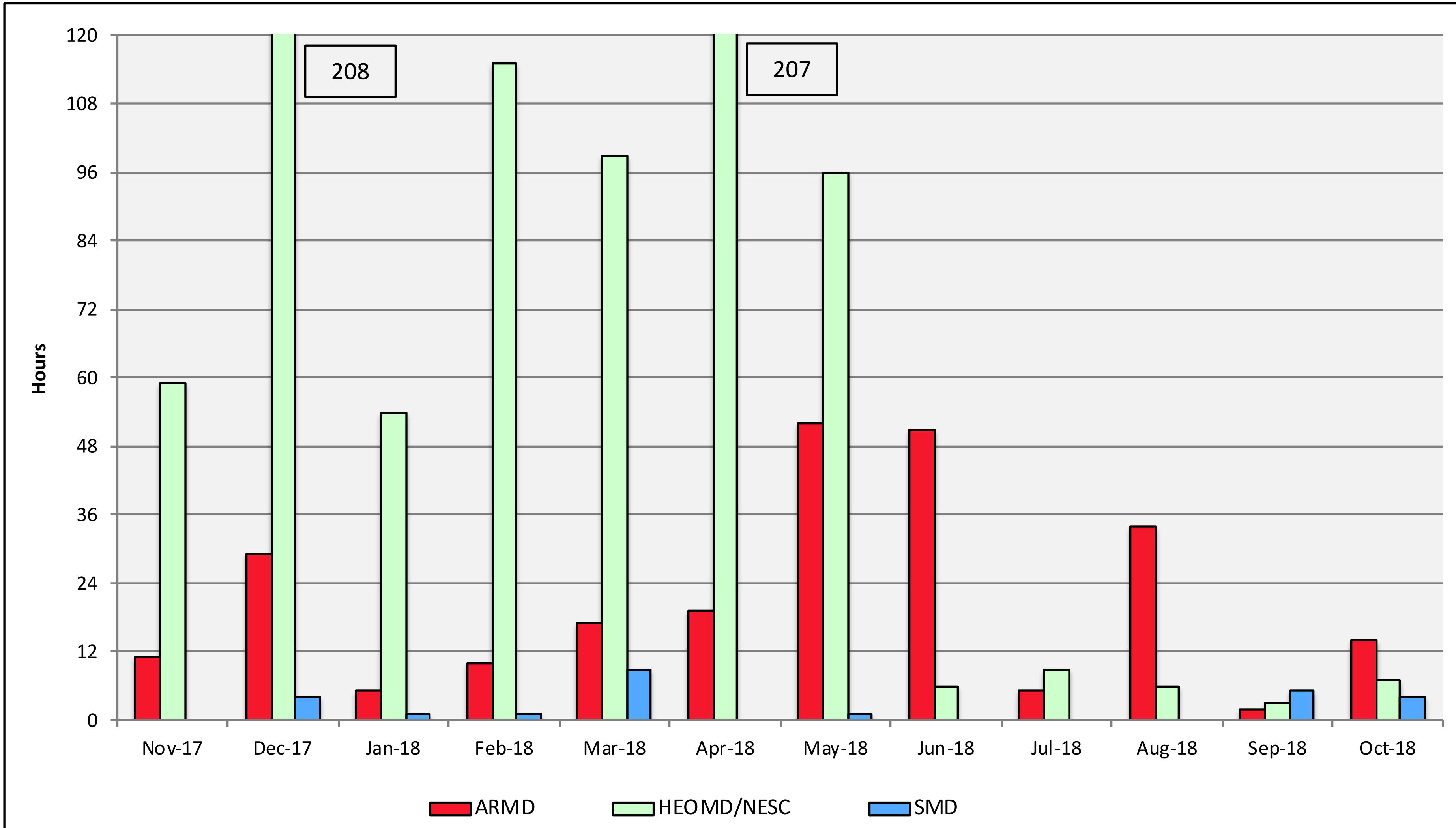
Endeavour: Monthly Utilization by Size and Mission



Endeavour:
Monthly Utilization by Size and Length



Endeavour: Average Time to Clear All Jobs



Endeavour:
Average Expansion Factor