National Aeronautics and
Space Administration

HIGH-END COMPUTING CAPABILITY PORTFOLIO

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Successful Aitken LINPACK and HPCG Benchmarks

- With the recent installation of Aitken, HECC and HPE engineers ran the LINPACK and HPCG benchmarks to stress test the system and identify any faulty components prior to releasing the system for general user availability.
- Aitken has a theoretical peak performance of 3.684 petaflops, and the system achieved 2.376 PF on the LINPACK benchmark. This ranks the system at #103 on the June 2019 TOP500 list. On the HPCG benchmark, Aitken achieved 45.47 teraflops and ranks at #59 on the June 2019 HPCG list. Aitken was submitted for inclusion in the November 2019 TOP500 and HPCG lists.
- The benchmarks were run over a four-day period, and through extensive diagnostic tests identified more than a dozen marginal hardware components that were replaced prior to user release.
- The LINPACK and HPCG benchmarks are widely used to evaluate the performance of different supercomputing systems and provide two complementary viewpoints on how systems perform on different workloads.

**The Linpack and HPCG numbers are embargoed until Top 500 release.*

IMPACT: Running diagnostic tests on the Aitken supercomputer enables HECC to provide a stable and productive resource for users in all mission directorates.

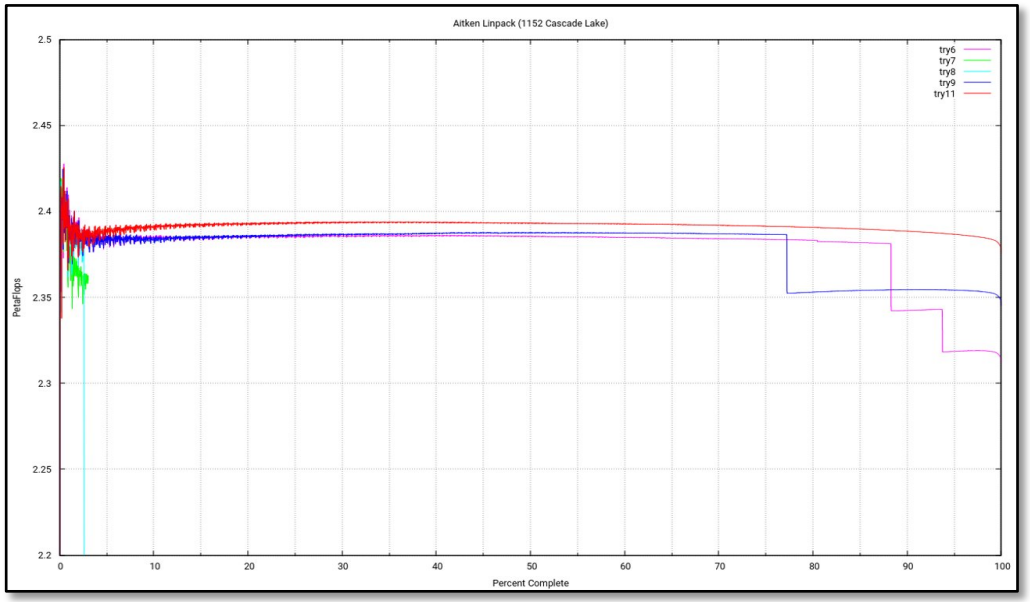
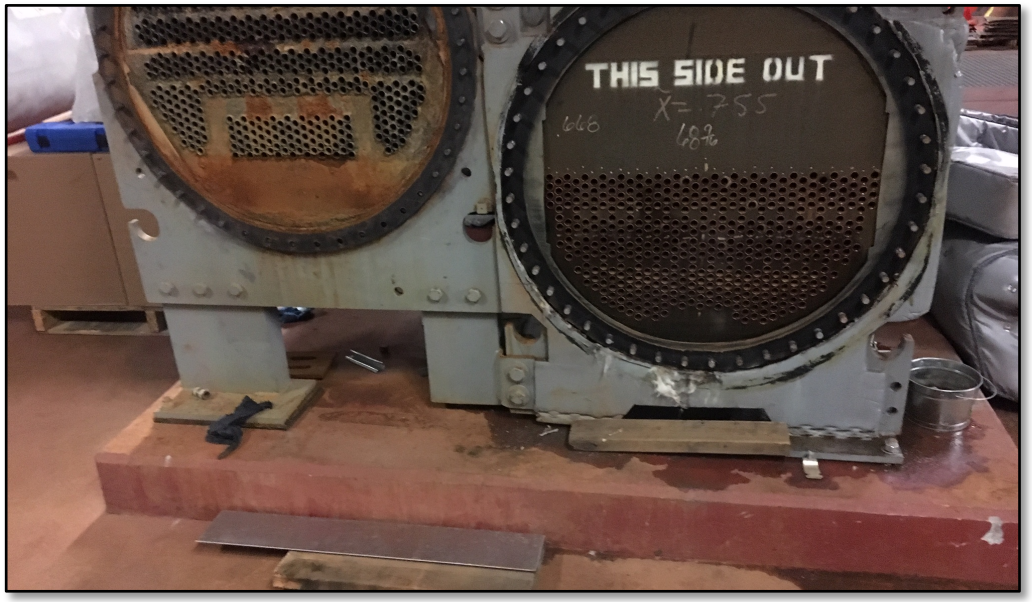


Chart showing the LINPACK runs on the Aitken supercomputer, with three successful runs. The last run was completed without errors and resulted in a 2.376-petaflop performance. The two other runs had hardware errors that significantly impacted the benchmark run. Each successful run takes approximately 9.5 hours to complete.

NAS Facility Cooling System Returns to Full Capacity

- Chiller #1 in the Building N258 cooling system was repaired and returned to service in October. All four 450-ton chillers at the NAS facility are now functional.
- The N258 cooling system requires three chillers to cool HECC resources. The cooling system is designed to have one chiller at-the-ready as a redundant chiller, should one of the three operating chillers fail. Until this month, the back-up chiller was out of service.
  - Chiller #1 operated infrequently over the last 18 months, with a refrigerant leak whose origin could not be determined. The chiller barrels were disassembled, and eddy current testing identified cracks in 11 of the nearly 1,000 chiller tubes as the cause of the refrigerant leak.
  - One condenser tube had a crack that was determined to be the main refrigerant leak, with 90–100% of the crack piercing through the wall thickness of the tube. The other 10 tubes had cracks at 40–70% through the wall thickness of the tube.
- Each of the cracked tubes were sealed with brass plugs that block water flow. Refrigerant can now fill the sealed tube, but the refrigerant is blocked from leaking into the water.
- With the return of Chiller #1, this crucial cooling system regains its redundant chiller and reduces the risk of an unplanned outage.

IMPACT: Cooling infrastructure that supports HECC resources has returned to design specifications to provide a resilient infrastructure providing consistent computer availability to NASA users.

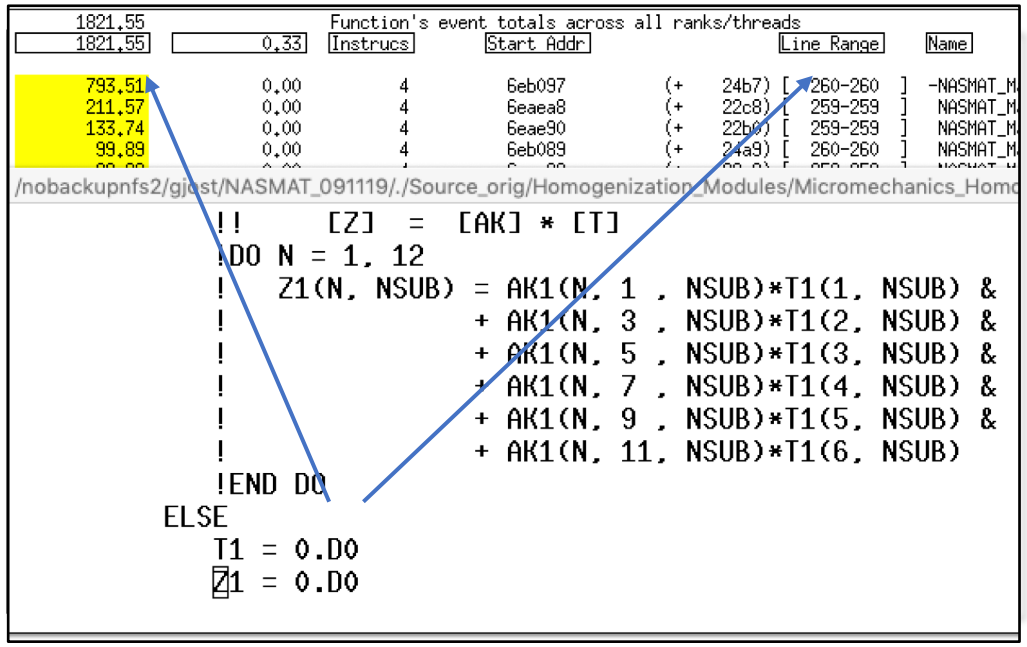


Chiller #1 end plates with the water tubes exposed. Water flows through the tubes as refrigerant flows over the exterior of the tubes. Brass plugs were inserted into the ends of the cracked tubes to block the flow of water and seal off the path of refrigerant leaking into the water. *Christopher Tanner, NASA/Ames*

Five Clicks Lead to 20x Performance Improvement in Multiscale Analysis Code

- HECC's Applications Performance and Productivity (APP) team improved the performance of the NASA Multiscale Analysis Tool (NASMAT) for high-fidelity experiments by a factor of more than 20x.
- The NASMAT code is being developed at Glenn Research Center.
  - It uses a multiscale analysis approach to bridge the gap between material science and structural engineering and is implemented in Fortran 2003.
  - The code is integrated within a larger framework but can also be run as a standalone application on a single CPU core.
- The NASMAT Team provided a standalone package and a set of test input data. The APP team then used the op_scope lightweight profiling tool, and with only five mouse clicks they identified:
  - Blocks with low performance caused by redundancies in the code.
  - Improvement opportunities involving memory layout changes.
- Addressing the identified issues resulted in a 20-fold improvement in code performance of the single-core test case.
- The APP team will continue to provide profiling support for future NASMAT developments.

IMPACT: Application program analysis tools are critical in ensuring effective use of HECC resources.



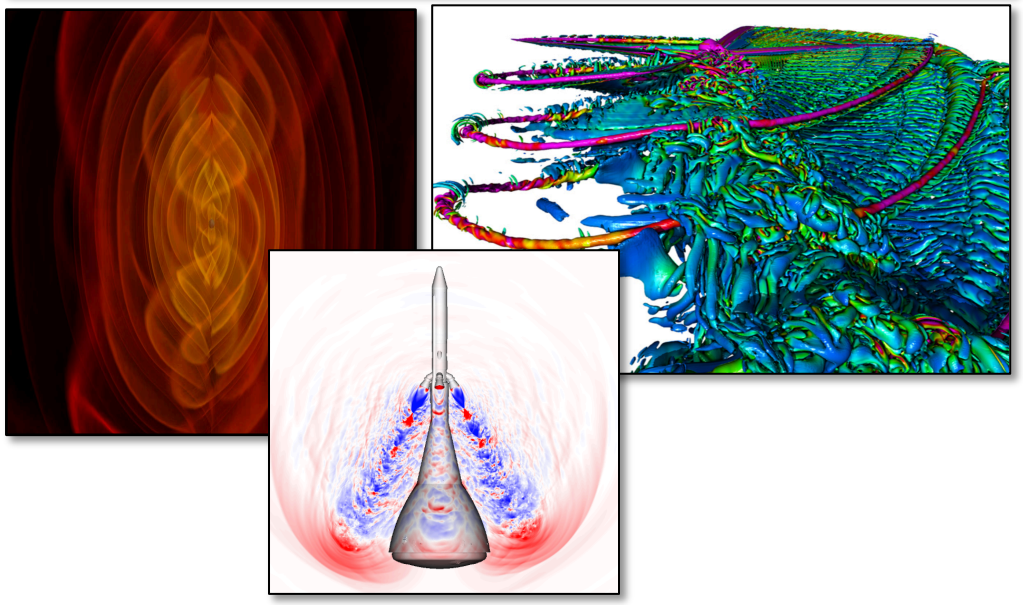
The op_scope tool indicates time-consuming functions and basic blocks with poor performance. A time-consuming basic block can be correlated to the corresponding source code via a simple mouse click, as shown in the screenshot above. This helps to quickly identify the culprits for poor performance.

New Allocation Period for Supercomputer Time Begins for NASA Mission Directorates

- The new allocation period for all NASA mission directorates began October 1.
  - Mission directorates awarded approximately 125 million Standard Billing Units (SBUs)* to 359 projects.
  - The Aeronautics Mission Directorate (ARMD) awarded more than 47 million SBUs to 149 projects.
  - The Human and Operations Mission Directorate, Space Technology Mission Directorate, and NASA Engineering and Safety Center collectively awarded more than 32 million SBUs to 112 projects.
  - The Science Mission Directorate awarded more than 36 million SBUs, with a surplus of 7.3 million SBUs to be awarded to future projects quarterly, to 142 projects.
- 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.

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

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

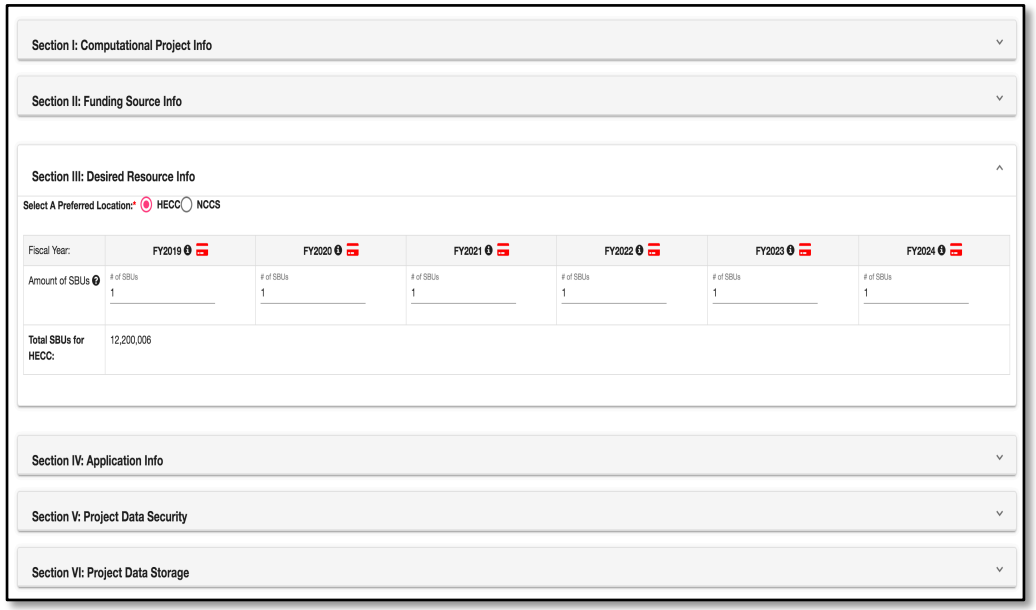


Images representing the variety of projects supported by HECC resources. Clockwise from top left: 1) Simulation of merging black holes and gravity waves; 2) UH-60 helicopter rotor simulation showing the 3D nature of the vortex wake; 3) Launch Abort Motor Qualification Motor 1 (QM-1) Static Test simulation with passive particles seeded at the nozzle exit and advected by the flow.

Request Management System Released for SMD

- The High-End Computing (HEC) program released a new in-house developed tool called the Request Management System (RMS) to partially replace REI eBooks. The initial October 1 release supports SMD, and there are plans to integrate the other mission directorates in later releases.
- The RMS tool enables new features such as:
  - Simplified processes for allocation requests, removing the eligibility request step from the process.
  - SMD users are now allowed to make multi-year allocation requests.
  - The in-house design allows for HEC ownership of the data.
- This milestone concluded the first of a multi-phase collaboration between HECC and NCCS User Services teams, with the next phase focusing on administrative enhancements.
  - The first phase supporting SMD serves as a prototype framework for the integration of HEOMD and ARMD, projected for FY2021.
- The new RMS log-in website is located at: https://request.hec.nasa.gov/login

IMPACT: Creating an in-house developed software for allocation requests allows more ownership of the data and simplification to the users process.

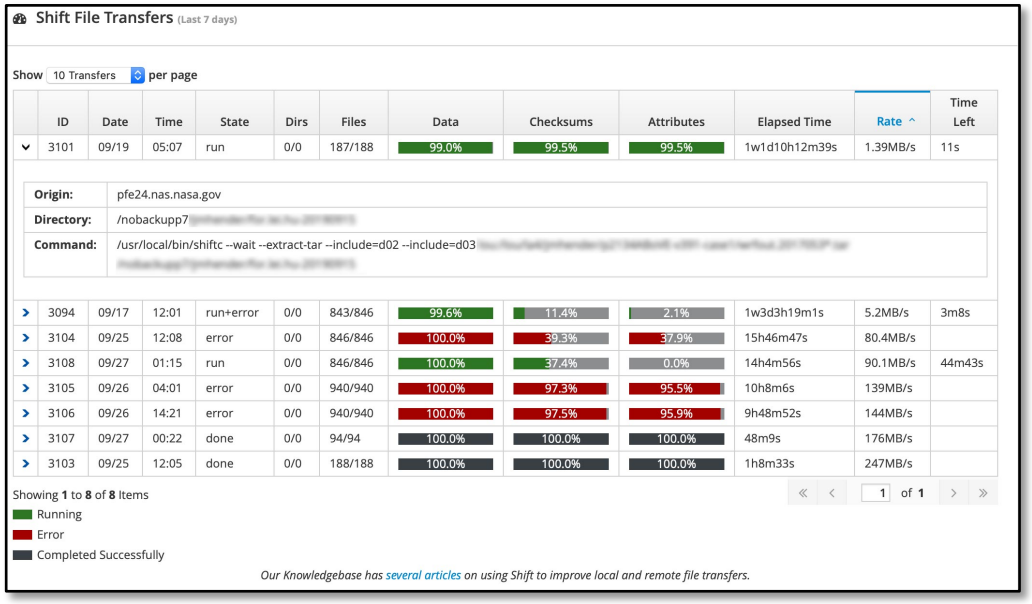


A screenshot from the new Request Management System demonstrating the multi-year allocation request process.

Tools Team Releases myNAS 1.1 to PIs and Users

- The HECC Tools team released a new version of the myNAS web portal (portal.nas.nasa.gov) to coincide with the beginning of the new operational year on October 1. This site provides principal investigators and users with near-real-time information on jobs and usage across all their GIDs.
- Several new features were introduced in this release, including:
  - Shift file transfer progress and detailed status information presented in a graphical table on the home page.
  - A home page widget that estimates the number of SBUs used by each GID since the official account year-to-date tally from the previous day.
  - Charts on the Accounts page that break down GID usage by HECC resource (Electra, Pleiades, and others).
- The Tools team collaborated with the Application Performance & Productivity team to update myNAS to reflect recent changes in the HECC environment, including the addition of Aitken and the change to a single HECC allocation for all resources.
- A new version of the myNAS Manager edition was also released this month, incorporating the single HECC allocation, Aitken data, and other improvements.

IMPACT: The myNAS portal provides users and principal investigators with an evolving set of tools to analyze and optimize their use of HECC resources.



The new Shift File Transfers table on the myNAS home page shows users detailed status for all their transfers over the previous seven days. Information includes number/size of files/directories, time elapsed, estimated time left, and data rate. The three progress bars show the status of each phase of the transfer, with colors indicating conditions such as running, warning, error, and complete.

New Monitors Increase the Mini-hyperwall's Visual Appeal

- HECC Visualization team members installed new mini-hyperwall monitors at the NAS facility to replace the old monitors that were failing.
- The new monitors have much thinner bezels (1.2 vs 2.3 millimeters) and have less-noticeable gaps between screens when a single image or video is displayed.
- The team also replaced monitor mounts with ones that include a fine-adjustment feature that makes it faster and easier to align the monitors.
- The mini-hyperwall is used extensively during NAS facility tours to demonstrate the importance of high-performance computing and modeling and simulation for NASA projects.
- In addition, the mini-hyperwall shipping crates were updated so the system can continue being used at the annual Supercomputing conference.
  - Two new crates hold the monitors.
  - The monitor frame crate was updated to accommodate the new monitor mounts.

IMPACT: Demonstrations on the mini-hyperwall locally and at the annual Supercomputing conference will be more attractive due to the new monitor's thinner bezels.

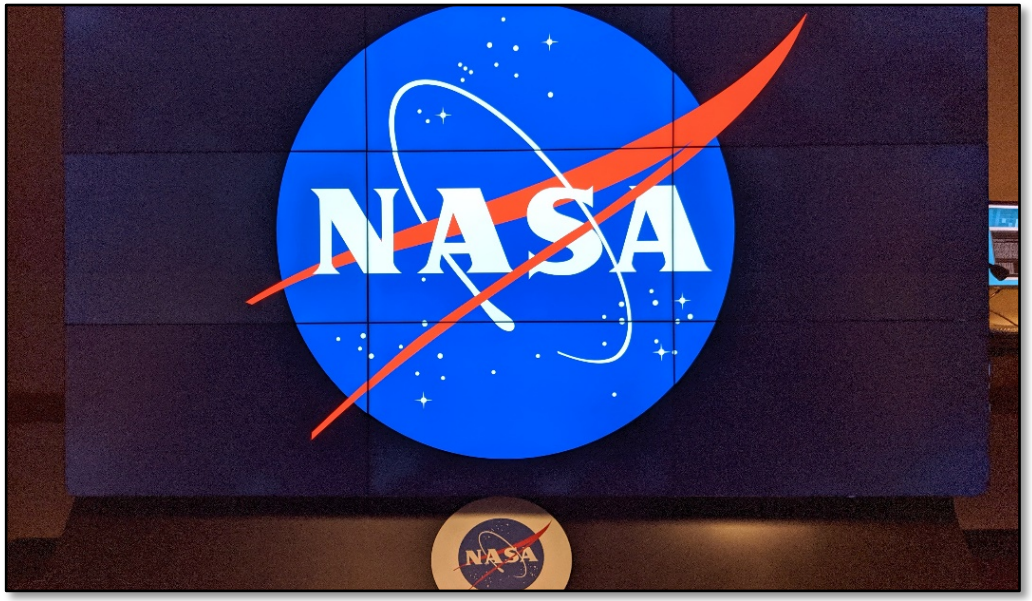


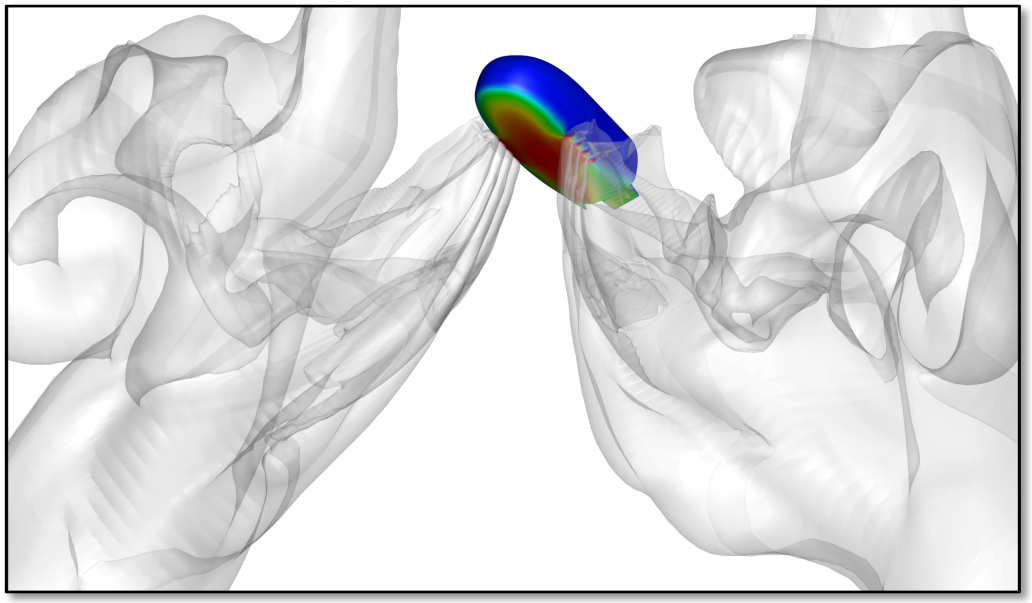
Photo of the mini-hyperwall monitors ready to be used for a demonstration. The new thinner bezels are so thin that they could be overlooked. *David Ellsworth, NASA/Ames*

Using Retrorockets for Human Exploration of Mars*

- The Descent System Studies team at NASA Ames is running computational fluid dynamics (CFD) simulations on Pleiades to study retropropulsion—a method for Entry, Descent, and Landing (EDL) that may be used in human missions to Mars.
- Aerospace engineers are considering using retropropulsion for these missions because EDL methods used in previous Mars missions are not scalable for delivering the massive payloads necessary for humans to survive on Mars.
- The simulation results help the researchers study the complex interactions between rocket plumes and incoming flow, providing important insights for analyzing the feasibility of design concepts for future Mars missions.
- CFD provides a valuable tool for analyzing different concept vehicles quickly and at relatively low costs. Engineers can change design parameters parameters to study the controllability and stability of a spacecraft using retropropulsion for powered descent and landing.

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

IMPACT: The knowledge and insights gained from these simulations are being applied to refine the design and architecture of future human exploration missions to Mars.



Visualization of the flow around a spacecraft with a mid lift-to-drag-ratio, with eight rocket engines firing to decelerate the vehicle. Colors indicate pressure (red is high, blue is low). The simulation illustrates how the expanding rocket plumes interact with the supersonic freestream, changing the surface pressure. *Chun Tang, NASA/Ames*

MSFC User Outreach Tour Aims to Improve Productivity

- In the final of three planned tours in 2019, a contingent of HECC staff visited users at Marshall Space Flight Center (MSFC) to highlight the project's extensive resources and services.
- The team held a successful discussion session with a very interactive group of more than 25 scientists, engineers, and partners who depend on HECC resources and services for their NASA projects.
  - Many attendees were Artemis users who expressed a strong interest in how to set up jobs for parallel execution of numerous serial jobs.
  - Attendees expressed interest in a simple reporting method for slow connections or Lustre issues that would not require response—this would be to help with spotting trends.
  - Users were also interested in getting allocations for more compute resources. The use of dedicated systems was discussed, as well as how the agency reserve SBUs are determined.
- The team will visit three different sites in Fiscal Year 2020.
- The presentation slides will be made available on the HECC website.

IMPACT: User outreach is critical to ensuring scientists and engineers make the most of their compute resources and give HECC staff a better understanding of users' needs.

Artemis team members attended the Marshall Space Flight Center user outreach tour. *Blaise Hartman, NASA/Ames*

HECC Facility Tours in October 2019

- HECC hosted 11 tour groups in September; guests learned about the agency-wide missions being supported by HECC assets, and also viewed the D-Wave 2000Q quantum system. Visitors this month included:
  - House Science Committee Democratic staffers Richard Obermann, John Piazza, and Kristin Kopshever.
  - Tristan Brown, Legislative Counsel, Office of Senator Gary Peters, Michigan; and Chris Beauregard, Policy Advisor, National Space Council.
  - Ron Thompson, Associate Chief Information Officer (ACIO) for Transformation and Data, and NASA's Chief Data Officer.
  - Colonel Jason Mello, Chief, Science and Engineering Division, Air Force Office of Scientific Research.
  - James Mazol, Policy Director, Aviation & Space and Security Subcommittees; Michael Reynolds, Deputy Policy Director; Darien Flowers and Joel Graham, Professional Staffers; Andrew Pate, Coast Guard Fellow; Sharmila Bhattacharya, NASA Senior Scientist; Coast Guard Liaisons Jillian Lamb, Sean Fullwood, Jack Souders.
  - Nancy Unger, Professor and Chair, Santa Clara University, who presented an Ames seminar, “An Illustrated Sampling of American LGBTQ + History: More than the Stonewall Riots!” in celebration of LGBT history month.

Piyush Mehrotra, NASA Advanced Supercomputing (NAS) Division Chief, gives Tristan Brown (right), Legislative Counsel, Office of Senator Gary Peters (Michigan), a tour of the Quantum Lab.
Gina Morello, NASA/Ames

Papers

- "**Toward Ultralight High Strength Structural Materials via Collapsed Carbon Nanotube Bonding**," B. Jensen, et al., Carbon, vol. 156, October 1, 2019. * https://www.sciencedirect.com/science/article/pii/S0008622319310048
- "**Exploring the Atmospheric Dynamics of Extreme Ultra-Hot Jupiter KELT-9b Using TESS Photometry**," I. Wong, et al., arXiv:1901.01607 [astro-ph.EP], October 3, 2019. * https://arxiv.org/abs/1910.01607
- "**Can an Unobserved Concentration of Magnetic Flux Above the Poles of the Sun Resolve the Open Flux Problem?**" P. Riley, et al., The Astrophysical Journal, vol. 884, no. 1, October 8, 2019. * https://iopscience.iop.org/article/10.3847/1538-4357/ab3a98/meta
- **"Ice Shelf Basal Melt Rates from a High-Resolution Digital Elevation Model (DEM) Record for Pine Island Glacier, Antarctica**," D. Shean, et al., The Cryosphere, vol. 13, issue 10, October 10, 2019. * https://www.the-cryosphere.net/13/2633/2019/
- "**Numerical Study of a Turbulent Separation Bubble with Sweep**," G. Coleman, C. Rumsey, P. Spalart, Journal of Fluid Mechanics, vol. 880, October 10, 2019. * https://www.cambridge.org/core/journals/journal-of-fluid-mechanics/article/numerical-study-of-a-turbulent-separation-bubble-with-sweep/0C6D0C288CE94659FFD899B3B35699B9

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

Papers (cont.)

- "**Exploring Plasma Heating in the Current Sheet Region in a Three-Dimensional Coronal Mass Ejection Simulation**," K. Reeves, et al., arXiv:19010.05386 [astro-ph.SR], October 11, 2019. * https://arxiv.org/abs/1910.05386
- "**Entropy Rain: Dilution and Compression of Thermals in Stratified Domains**," E. Anders, D. Lecoanet, B. Brown, The Astrophysical Journal, vol. 884, no. 1, October 11, 2019. * https://iopscience.iop.org/article/10.3847/1538-4357/ab3644
- "**Meridional Flows in the Disk Around a Young Star**," R. Teague, J. Bae, E. Bergin, Nature, vol. 574, October 16, 2019. * https://www.nature.com/articles/s41586-019-1642-0
- "**Interactions Between Asteroid Fragments During Atmospheric Entry**," P. Register, et al., Icarus, vol. 337, October 24, 2019. * https://www.sciencedirect.com/science/article/pii/S001910351930452X
- "**Prior Biosphere Model Impact on Global Terrestrial CO_2 Fluxes Estimated from OCO-2 Retrievals**," S. Philip, et al., Atmospheric Chemistry and Physics, vol. 19, issue 20, October 28, 2019. * https://www.atmos-chem-phys.net/19/13267/2019/
- "**Electron Trapping in the Coma of a Weakly Outgassing Comet**," C. P. Sishtla, et al., Physics of Plasmas, vol. 26, issue 10, October 28, 2019. * https://aip.scitation.org/doi/full/10.1063/1.5115456

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

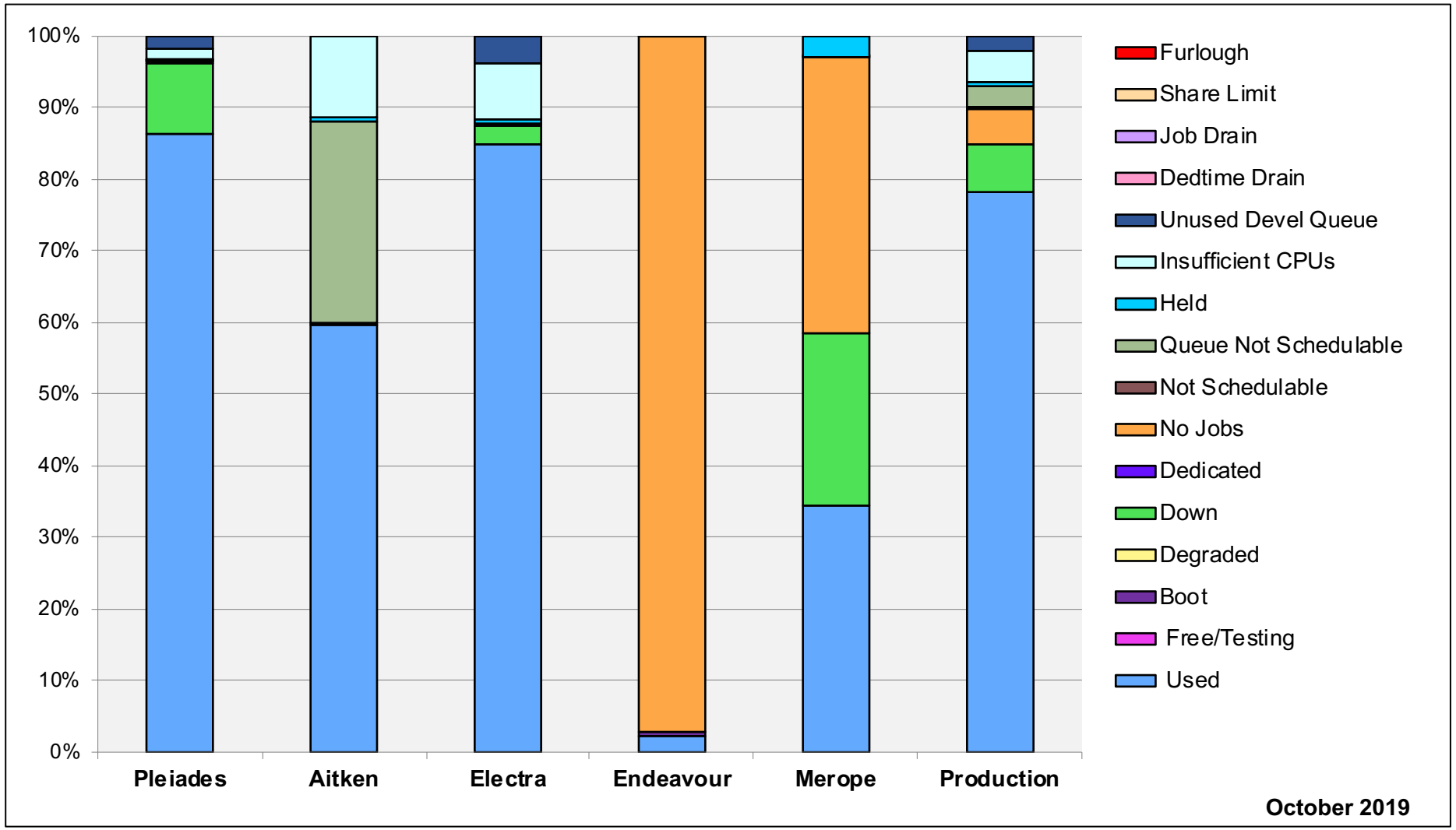
News and Events

- **Predictive Science Researchers Utilize XSEDE Supercomputers for Test Runs of an Eclipse**, *HPCwire*, October 8, 2019—Predictive Science Inc. researchers ran their final model predicting the details of the July 2, 2019 total eclipse of the sun on the Pleiades supercomputer. https://www.hpcwire.com/off-the-wire/predictive-science-inc-researchers-rely-on-xsede-supercomputers-for-test-runs-of-the-total-eclipse/
  - Related: **How Scientists Used NASA Data to Predict Appearances of July 2 Eclipse**, *NASA Feature,* reported in the July 2019 HECC Monthly Report. https://www.nasa.gov/feature/how-scientists-used-nasa-data-to-predict-appearance-of-july-2-eclipse
- **Cascades of Gas Around Young Star Indicate Early Stages of Planet Formation**, *Carnegie Science*, October 16, 2019—New research reported in *Nature* utilized the Pleiades supercomputer to simulate the effects of three planets in the process of forming around a young star, revealing the source of their atmospheres. https://carnegiescience.edu/news/cascades-gas-around-young-star-indicate-early-stages-planet-formation
- **Google and NASA Achieve Quantum Supremacy**, *NASA Ames Press Release*, October 23, 2019—The advanced techniques needed for simulating quantum computations were developed with help from NASA Advanced Supercomputing Division experts and the Pleiades and Electra supercomputers. https://www.nasa.gov/feature/ames/quantum-supremacy

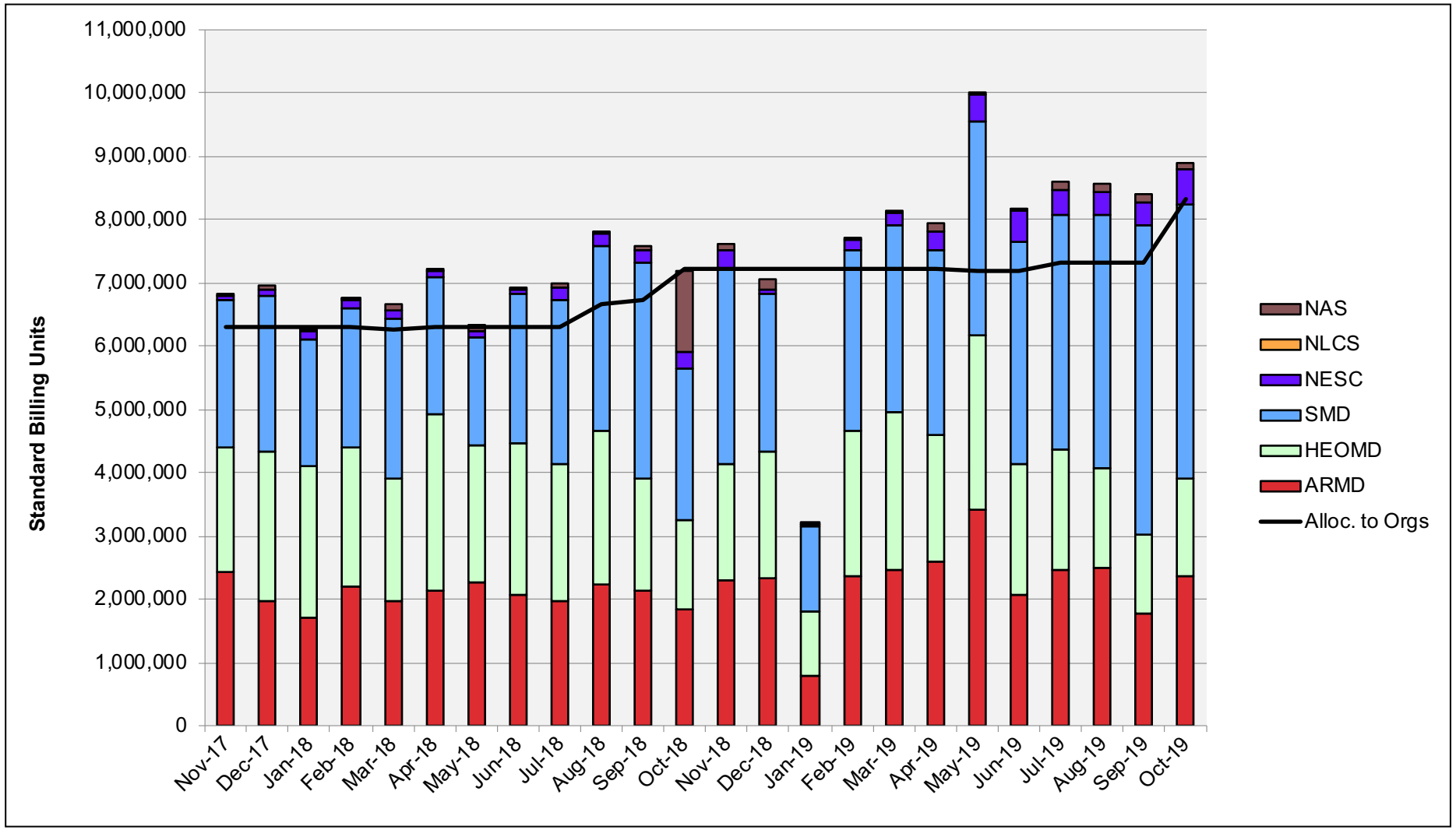
News and Events: Social Media

- **Top Posts from NAS**
  - Space Launch System booster separation dataset/video run on NAS supercomputers
    - Facebook: 443 users reached, 37 engagements
    - Twitter: 9 retweets, 21 likes
  - NASA Mars retropulsion research using HECC Visualization services and Oak Ridge National Lab's Summit supercomputer
    - Facebook: 2,161 users reached, 323 engagements
    - Twitter: 3 retweets, 8 likes
  - Solar weather simulation run on the Pleiades supercomputer
    - Facebook: 535 users reached, 49 engagements
    - Twitter: retweets 9, 15 likes

HECC Utilization



HECC Utilization Normalized to 30-Day Month



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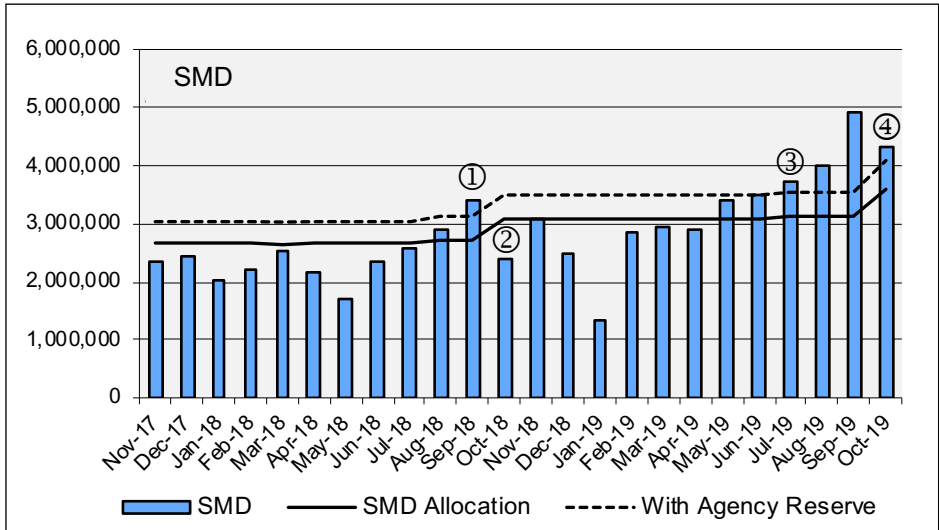
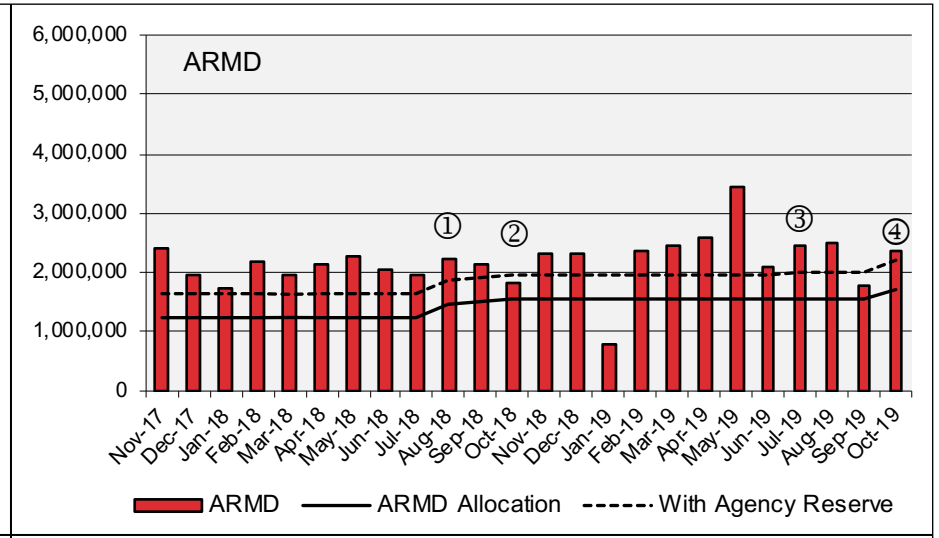
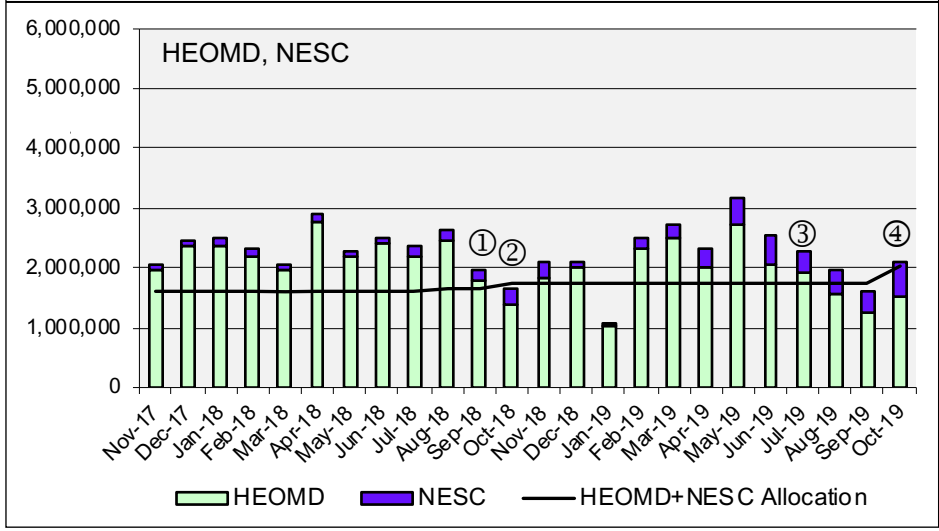






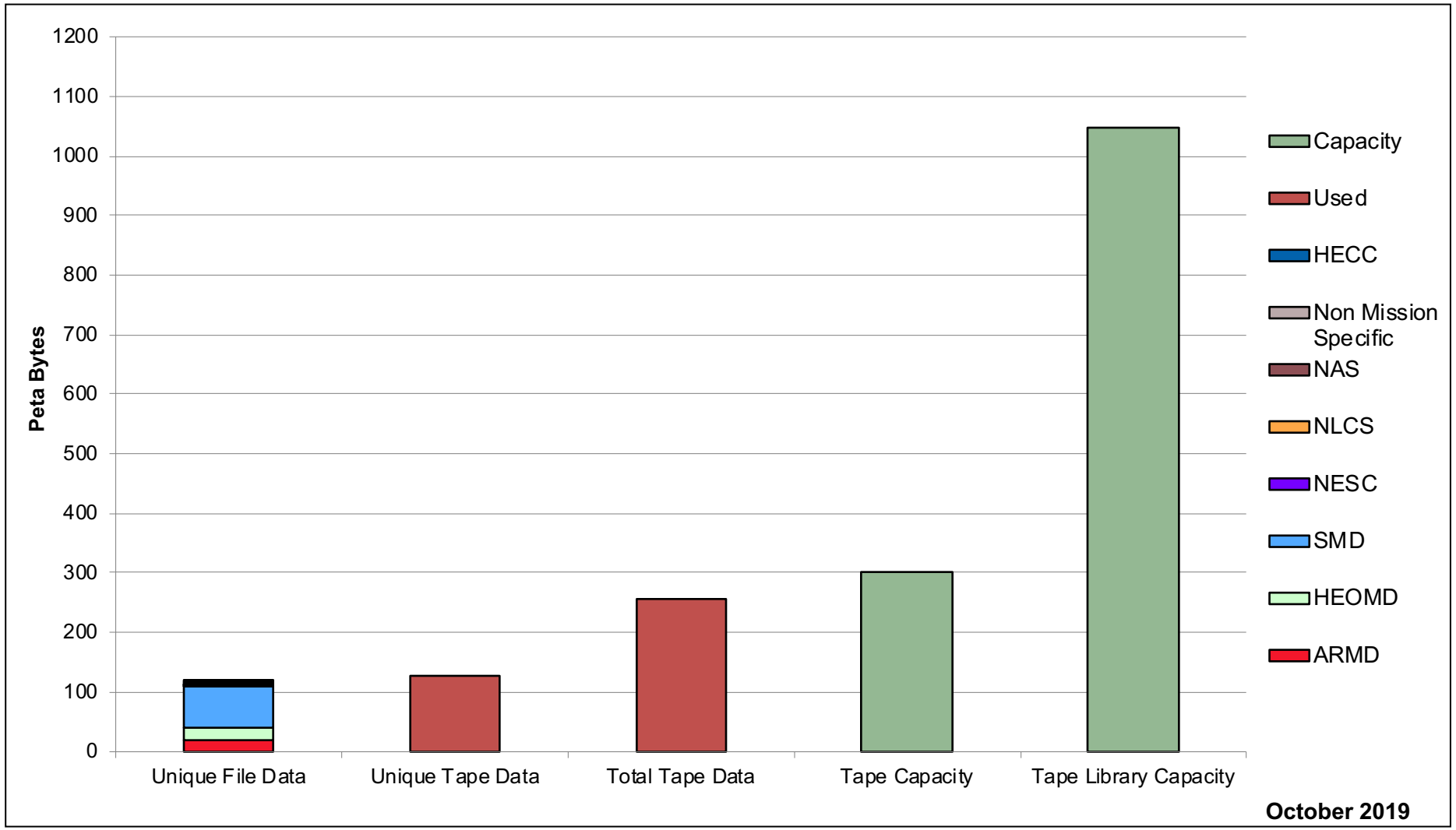
① 4 Skylake E cells (16 D Rack Equivalence) added to Electra

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

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

④ Skylake Tesla GPU V100 Nodes installed

Tape Archive Status



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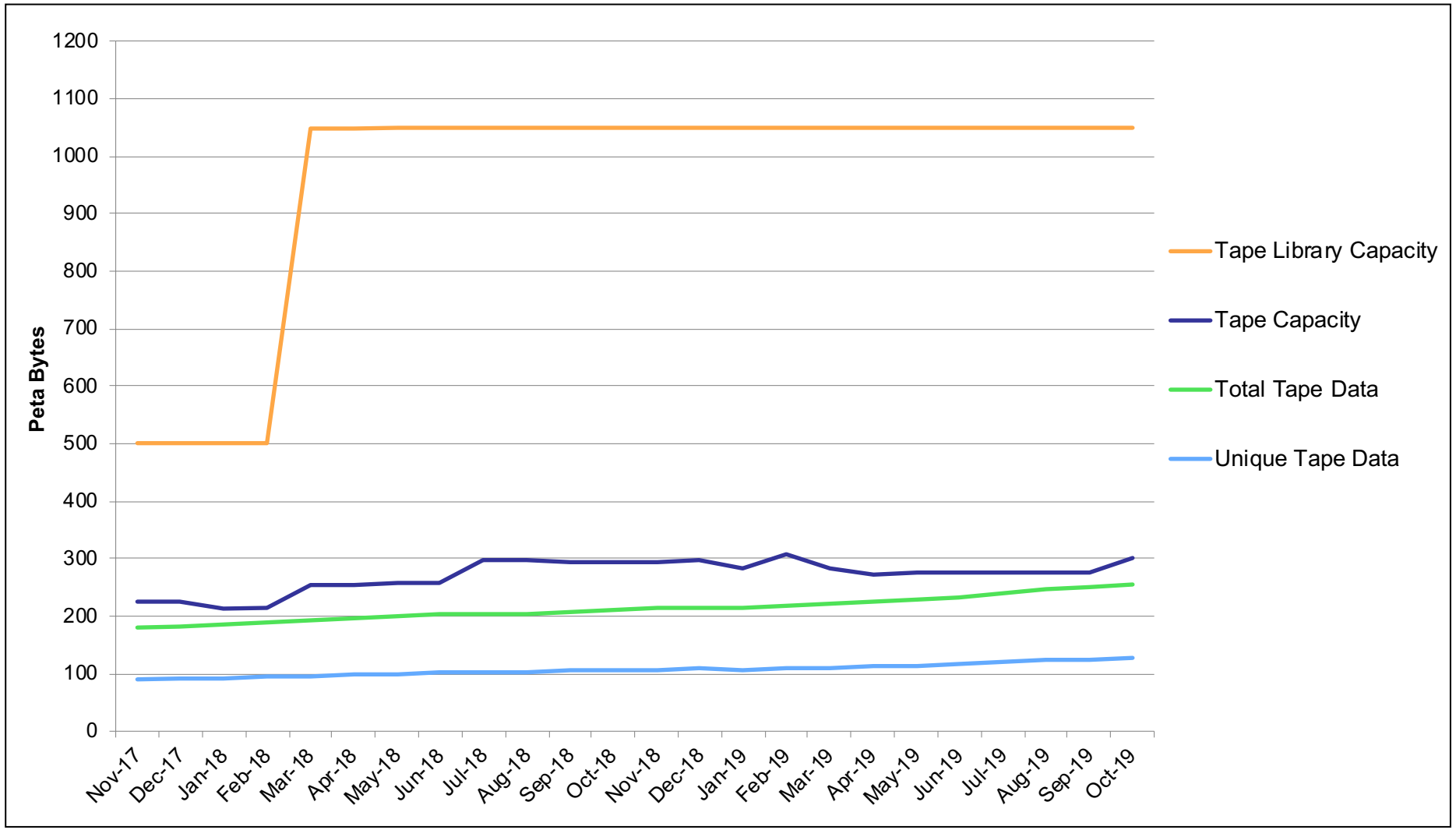
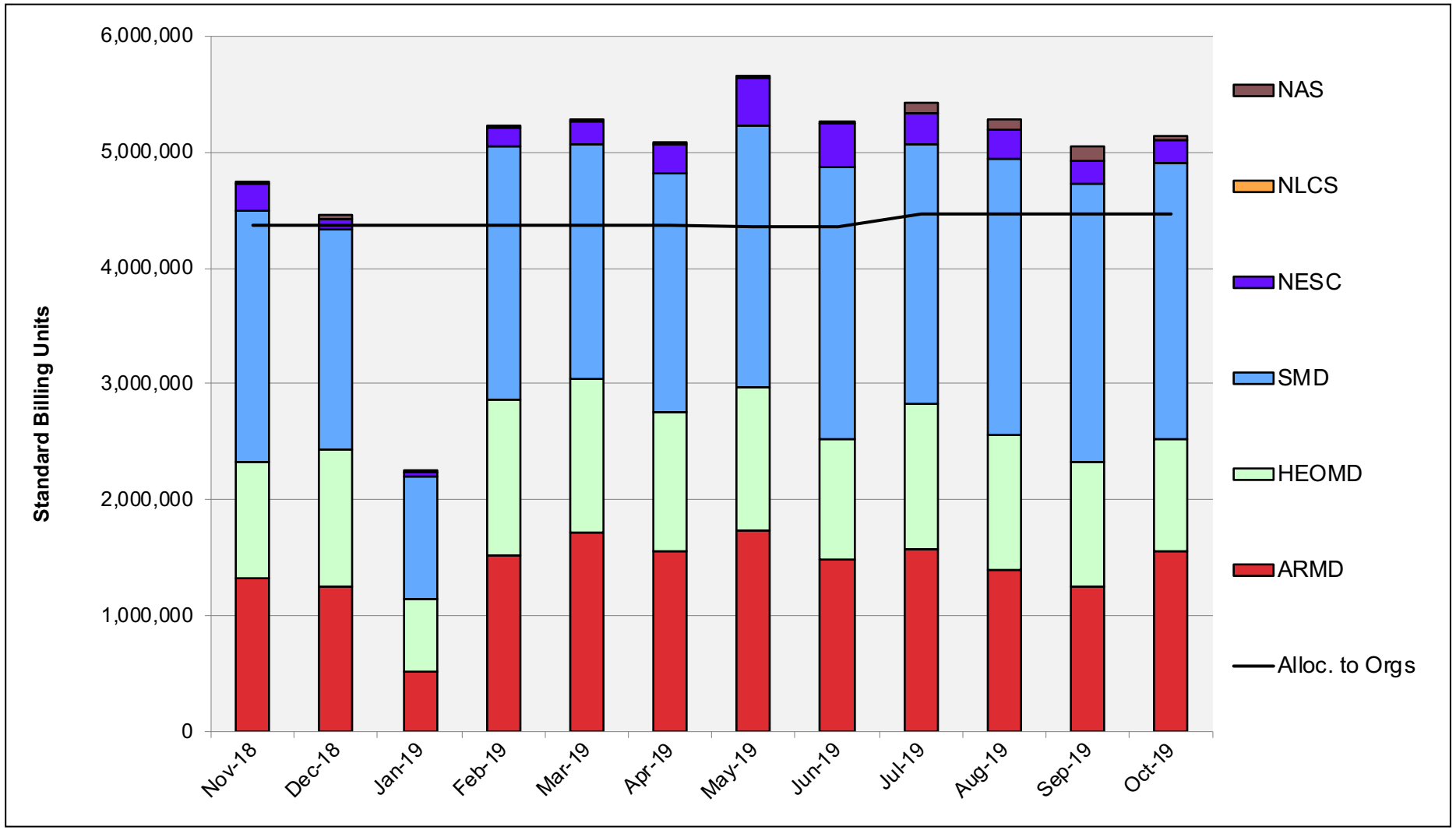
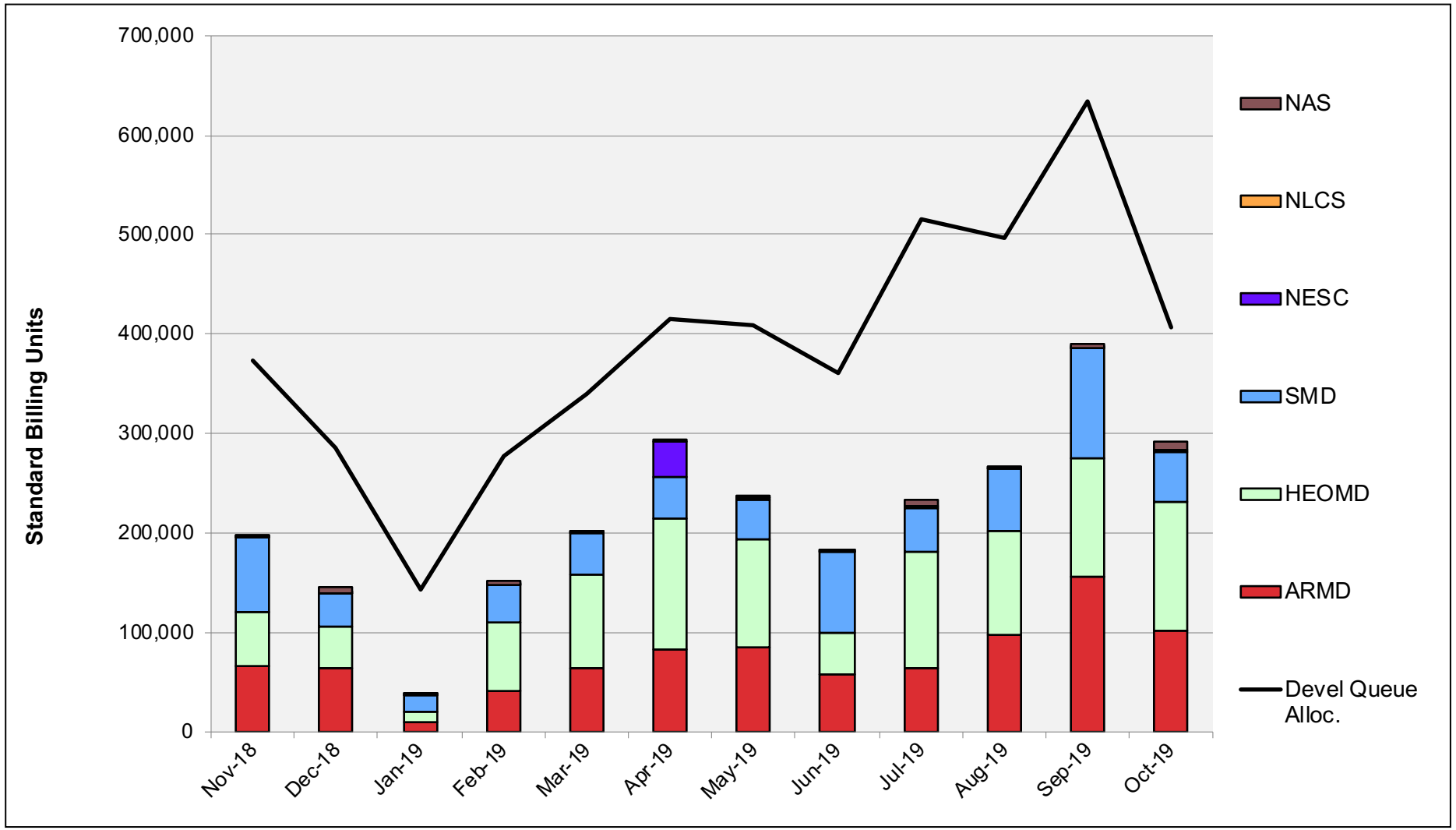


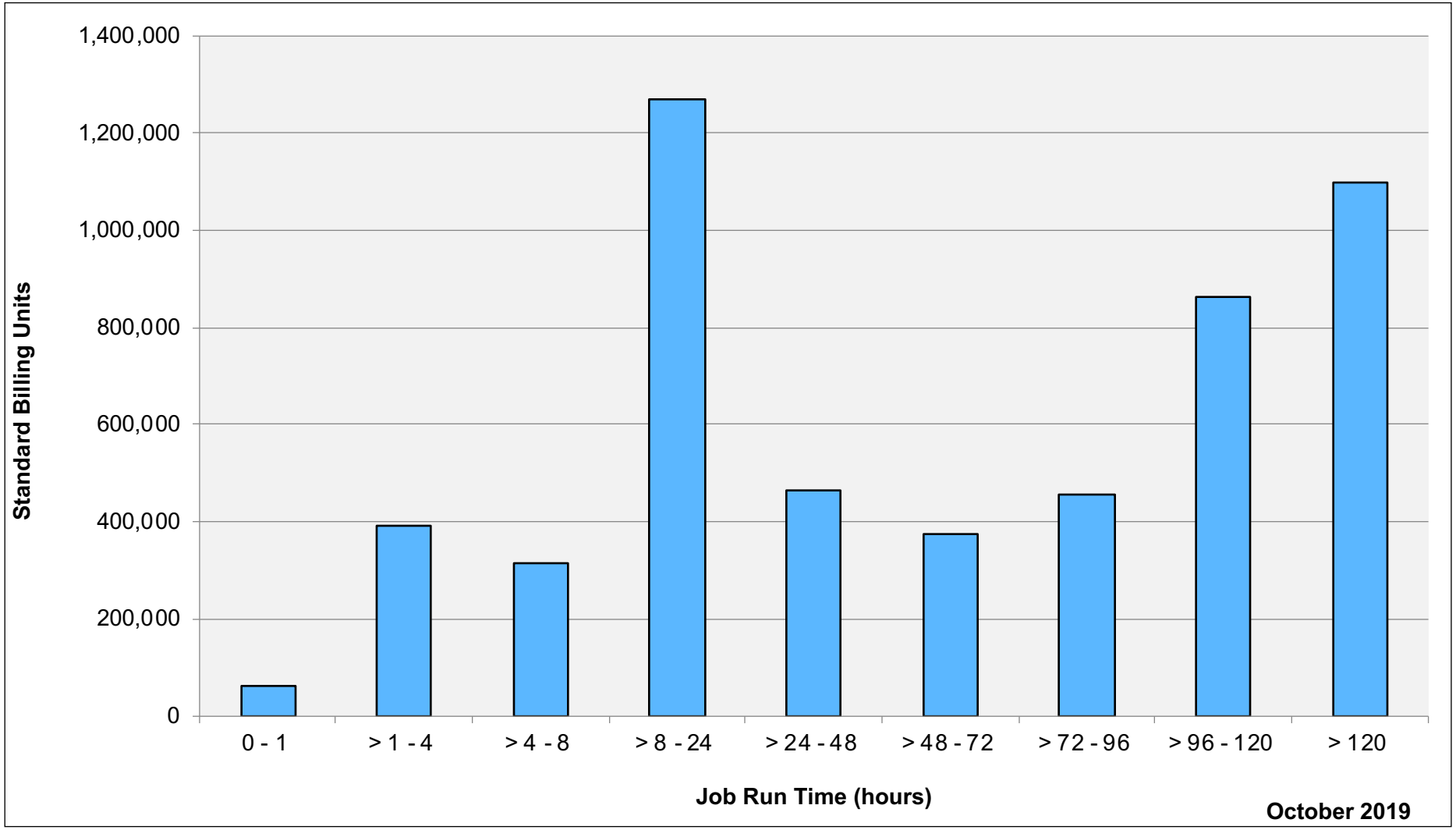
Pleiades: SBUs Reported, Normalized to 30-Day Month



Pleiades: Devel Queue Utilization



Pleiades: Monthly Utilization by Job Length



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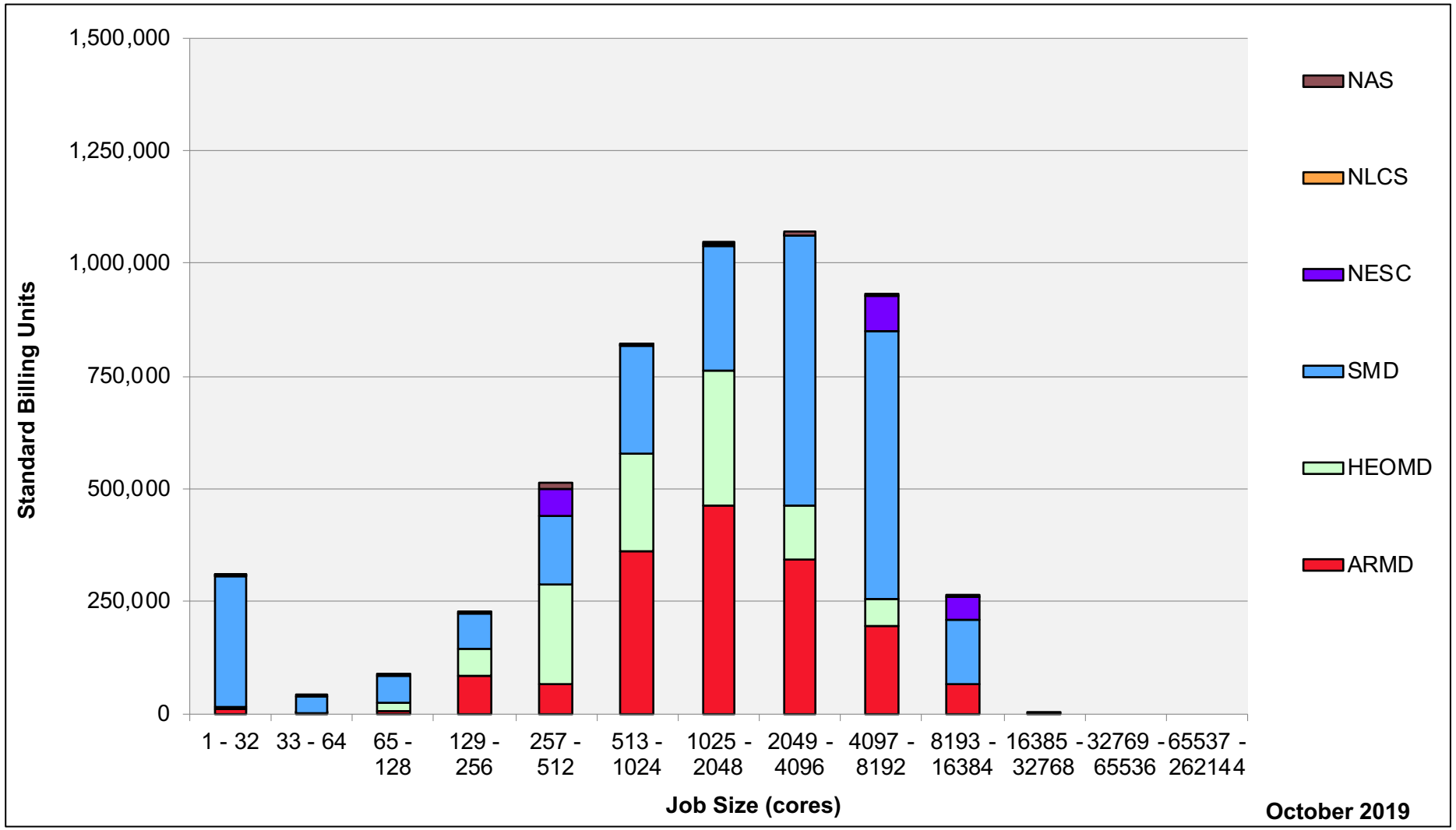
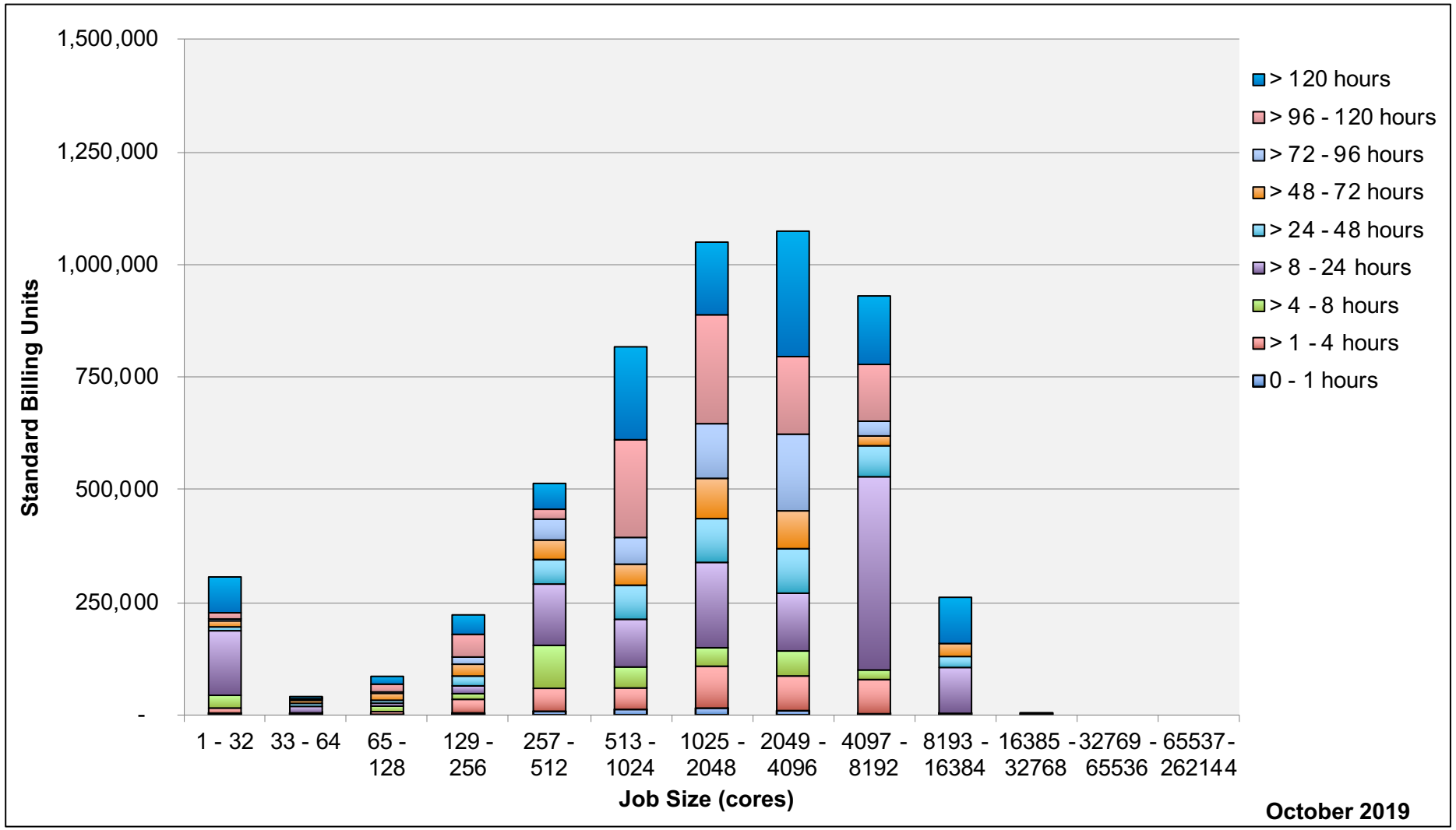
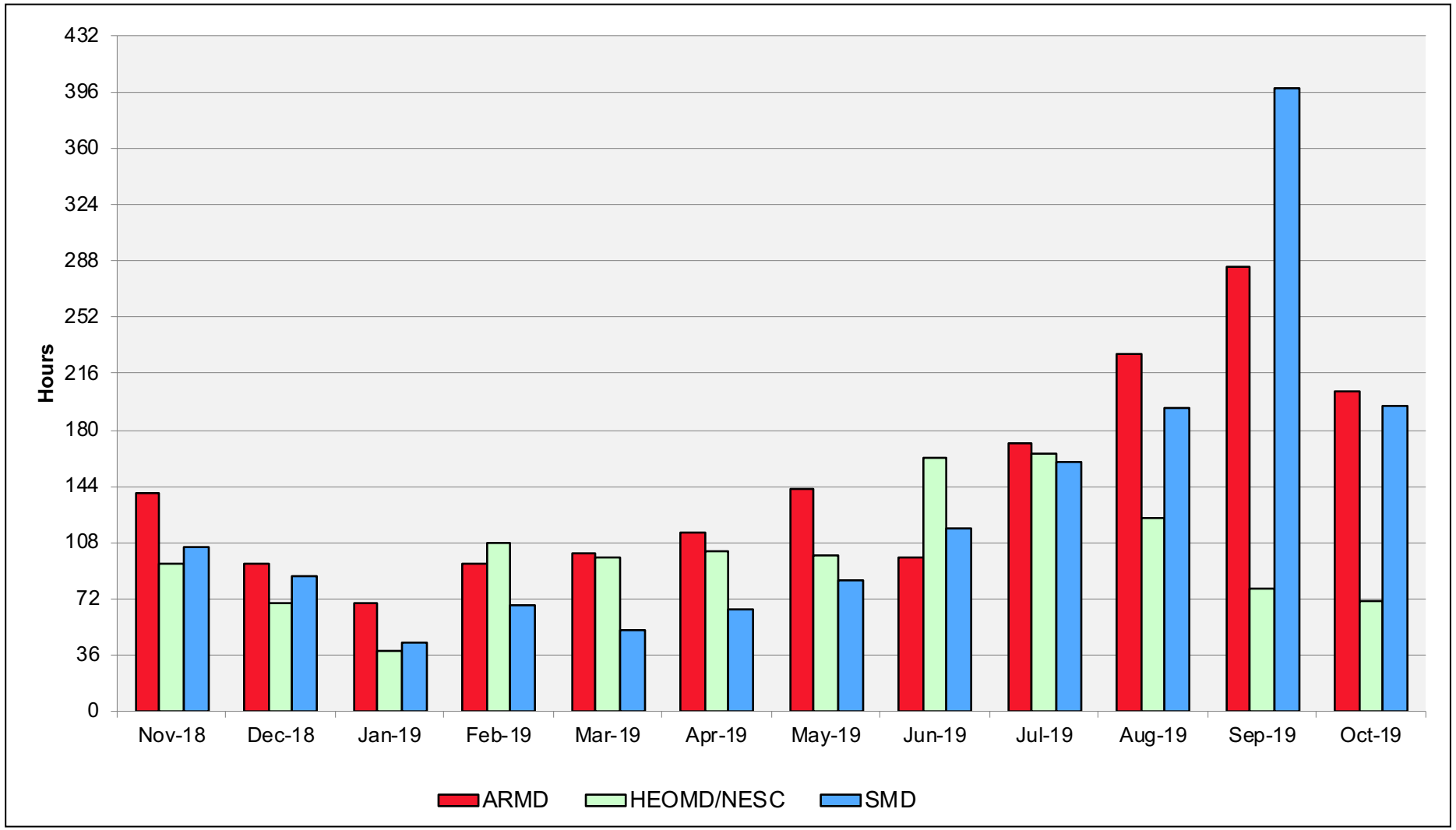


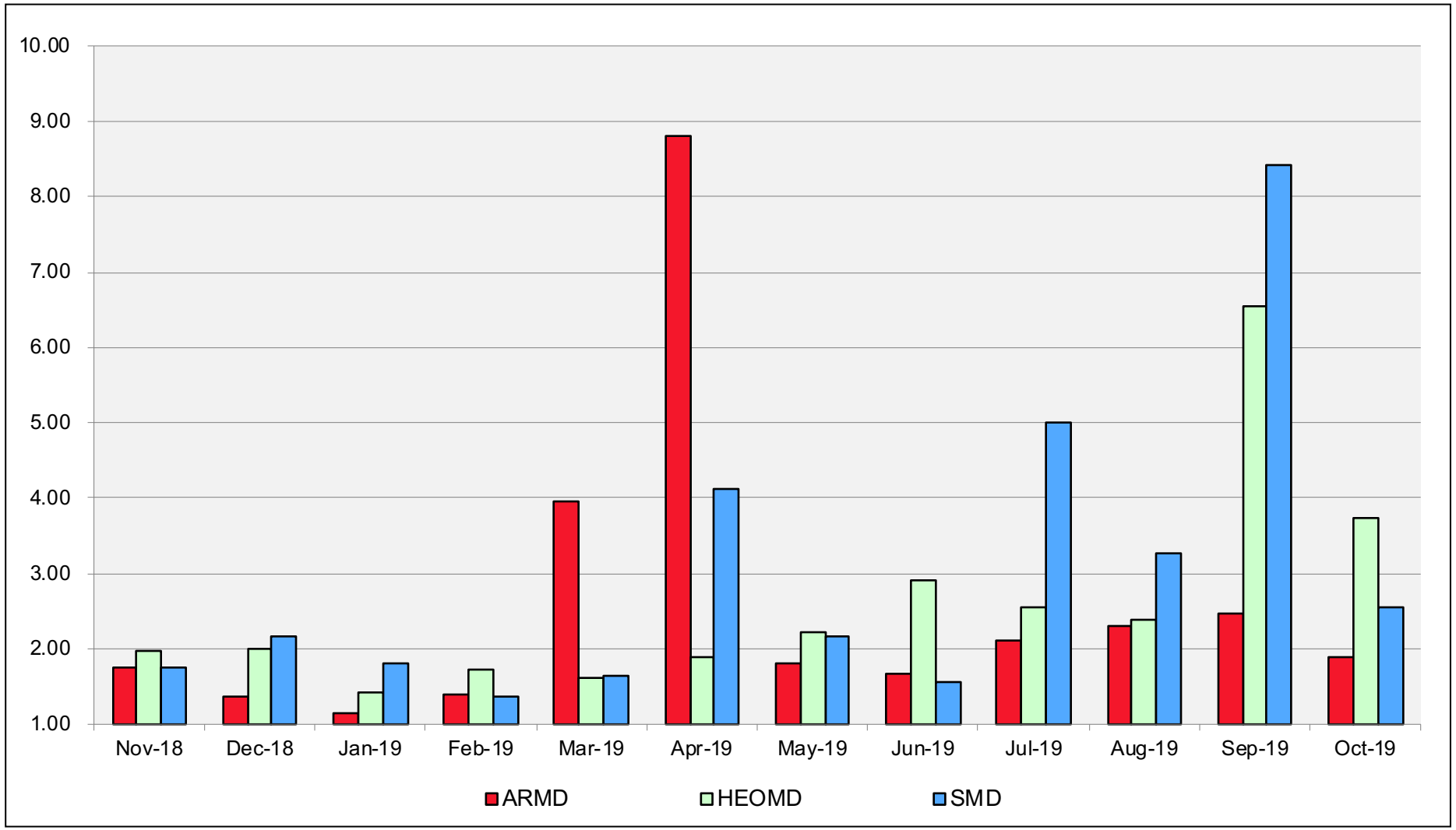
Pleiades: Monthly Utilization by Size and Length



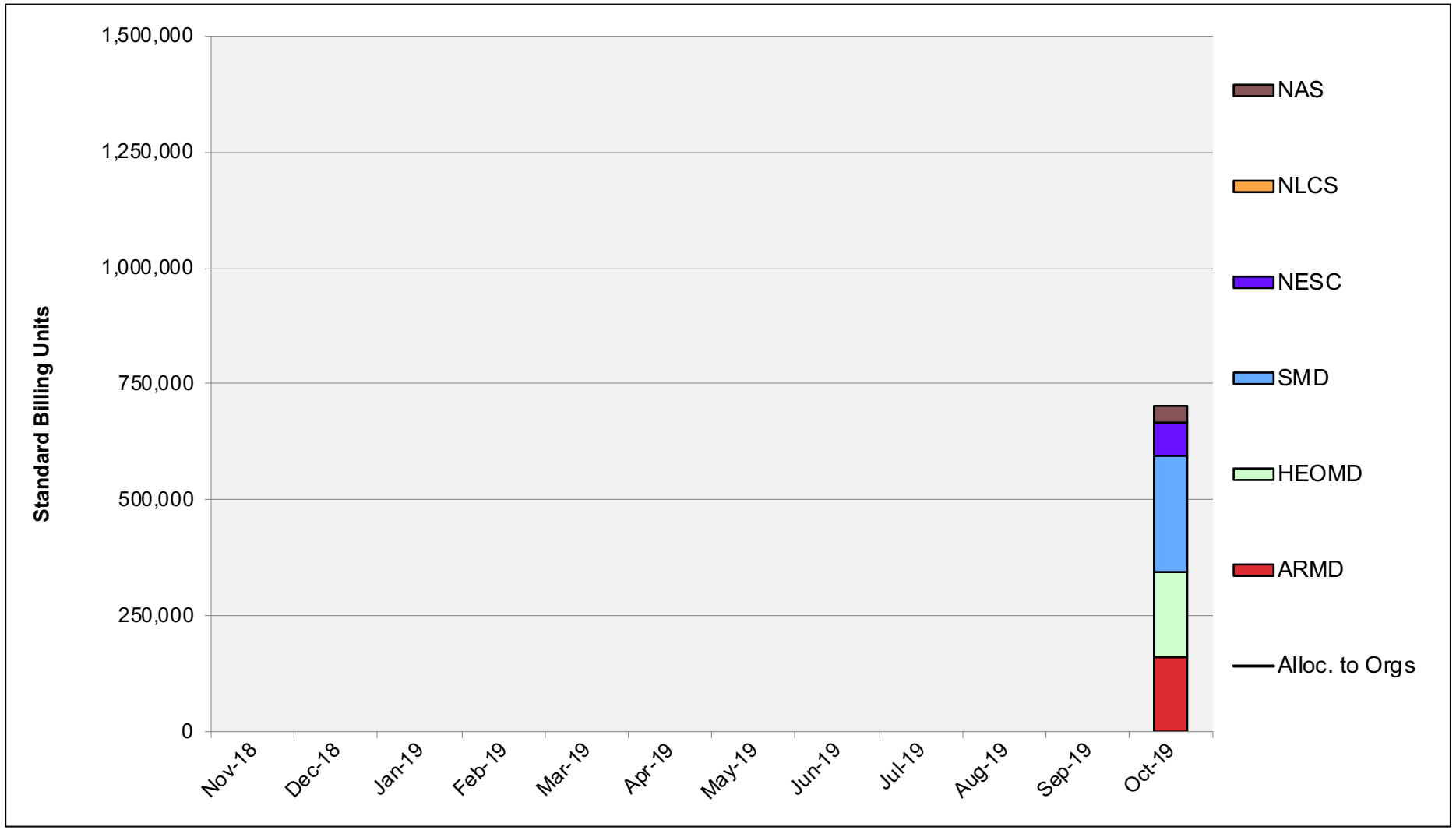
Pleiades: Average Time to Clear All Jobs



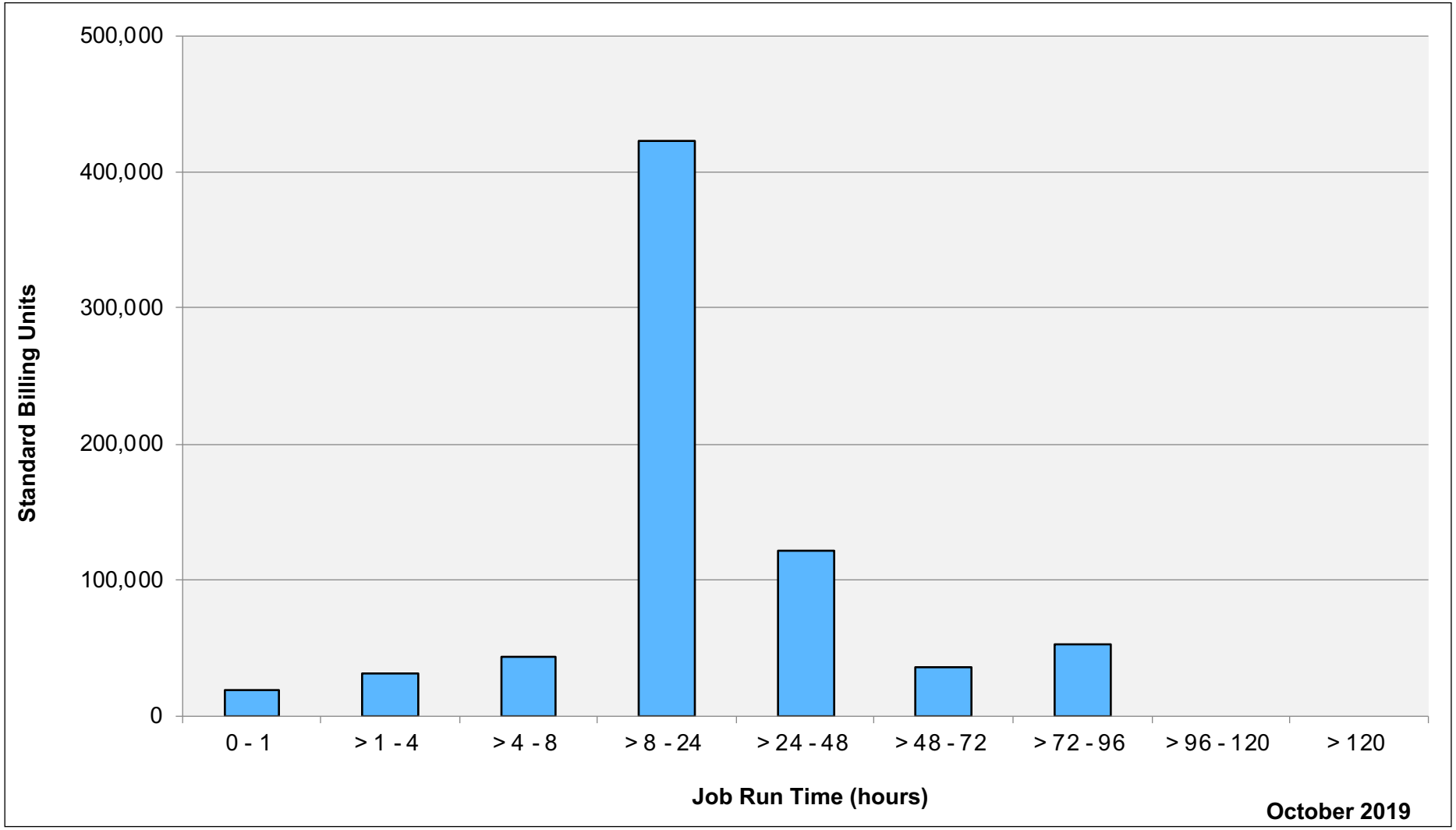
Pleiades: Average Expansion Factor



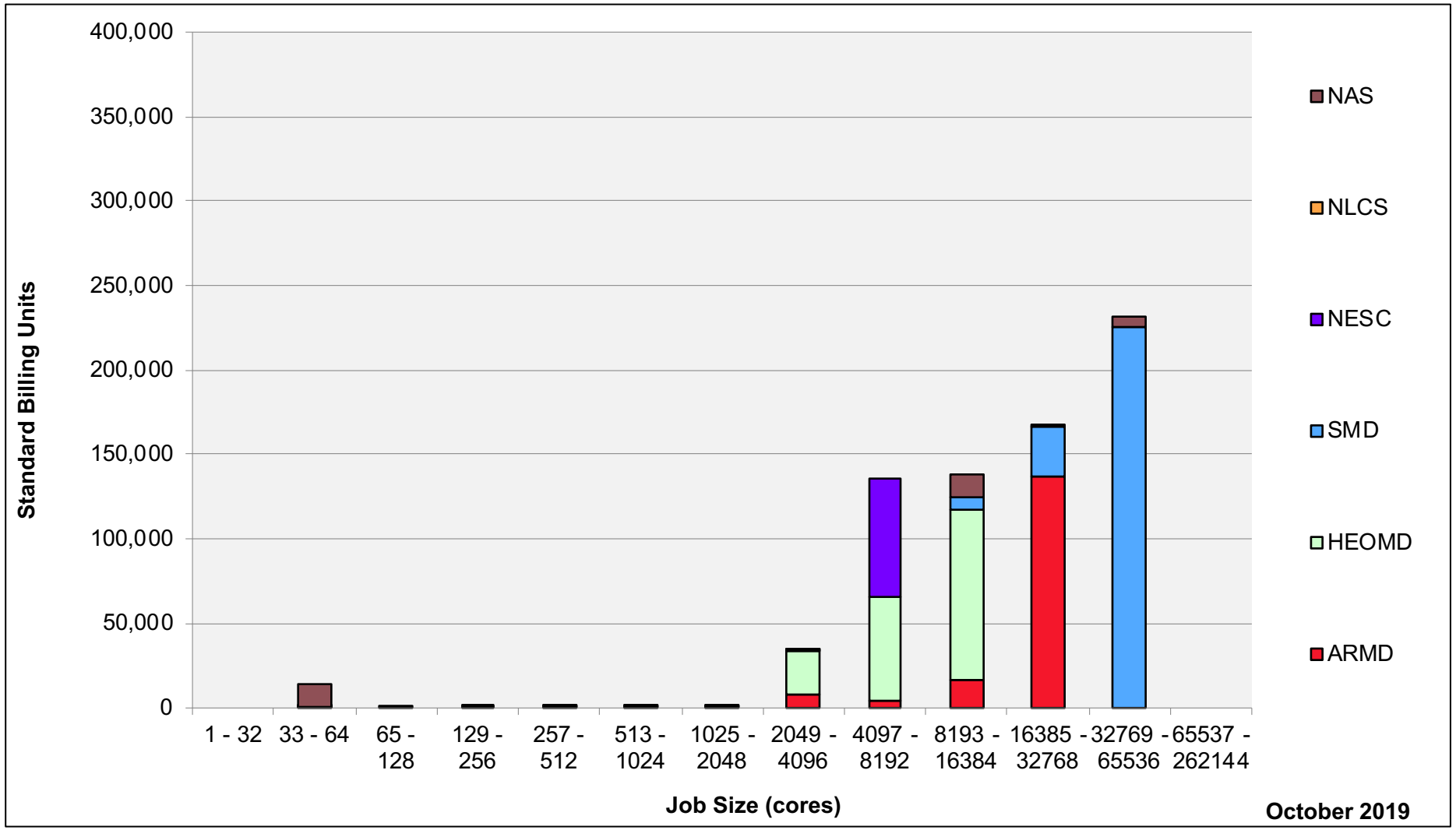
Aitken: SBUs Reported, Normalized to 30-Day Month



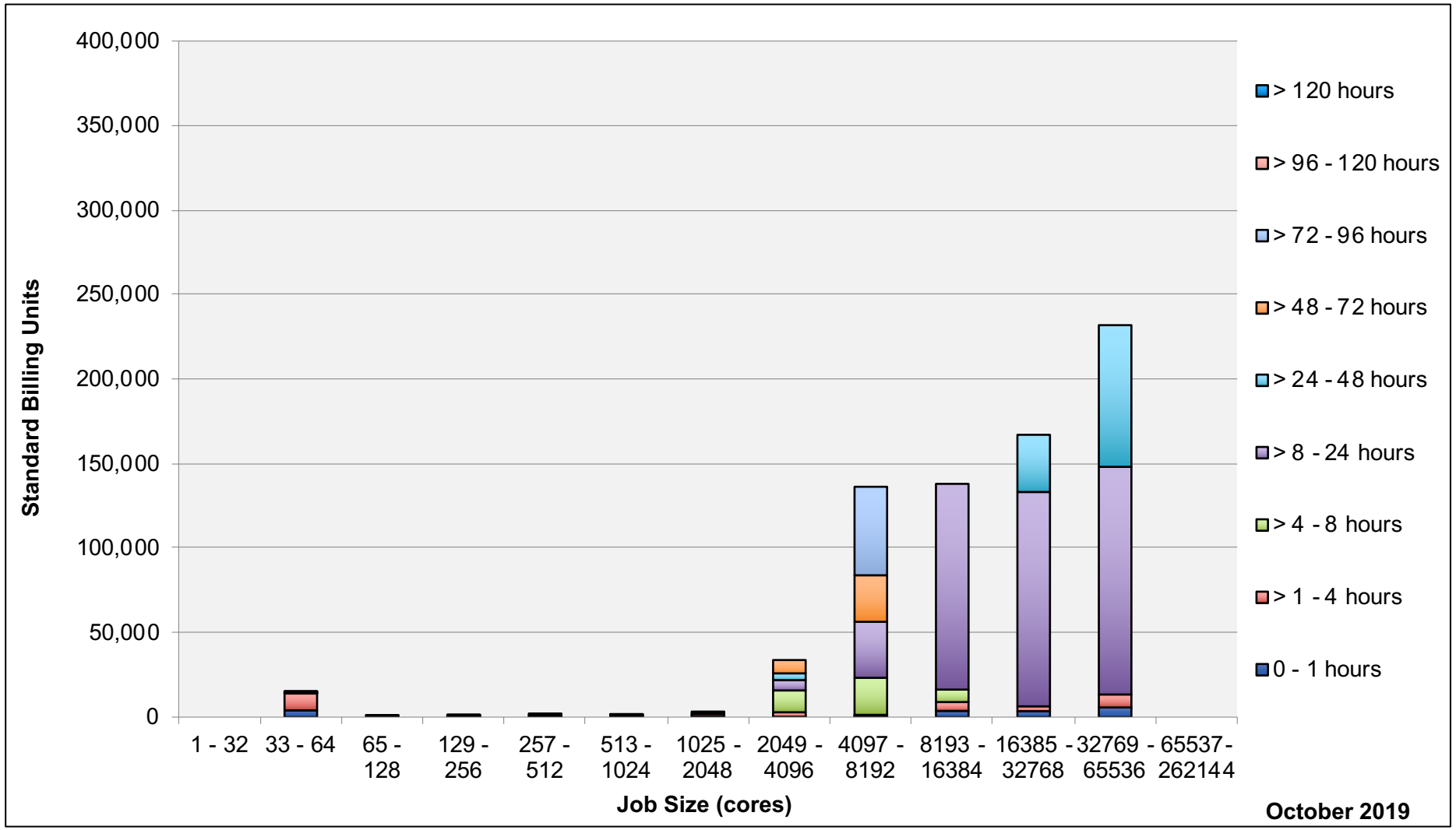
Aitken: Monthly Utilization by Job Length



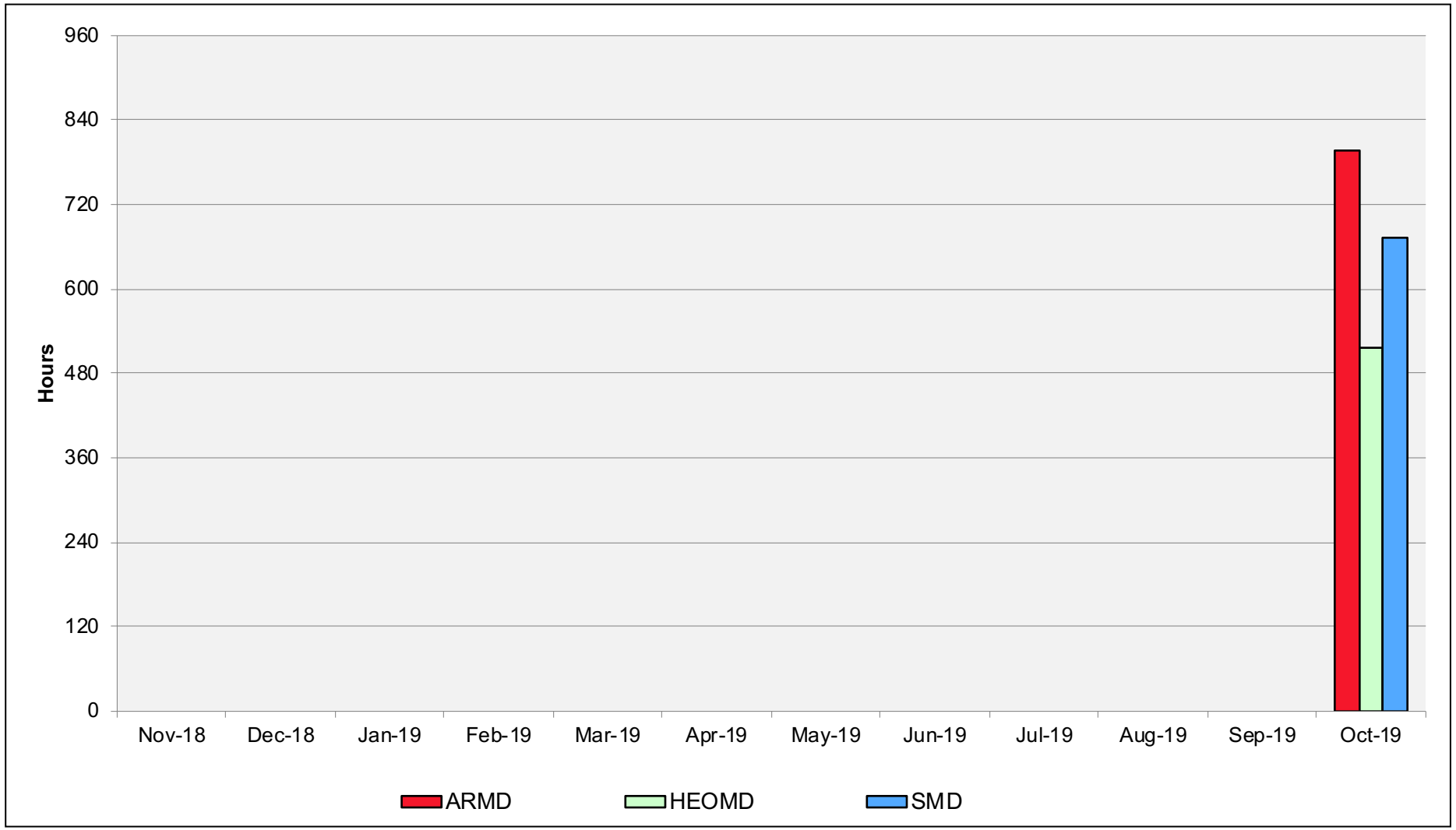
Aitken: Monthly Utilization by Job Length



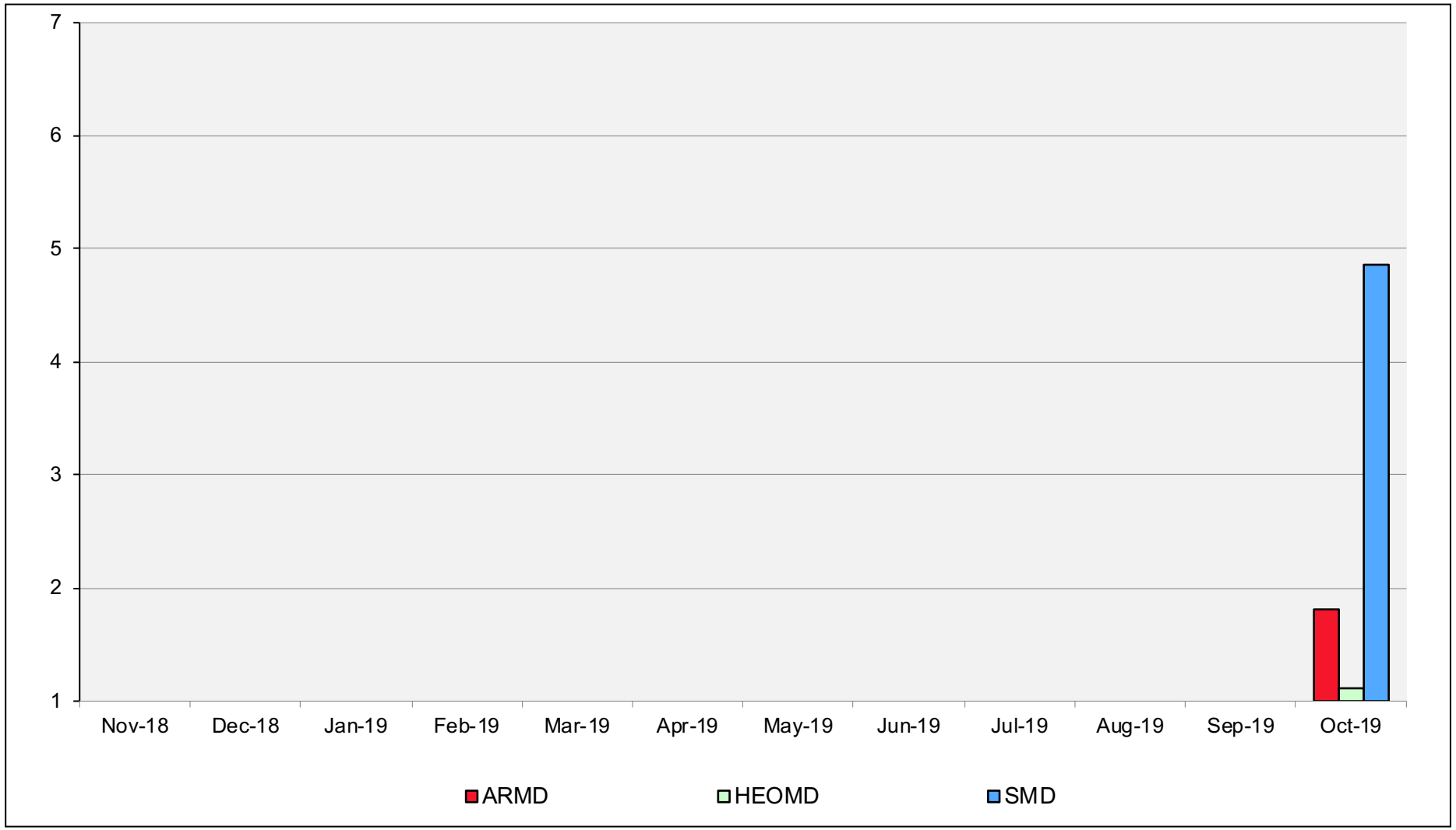
Aitken: Monthly Utilization by Size and Length



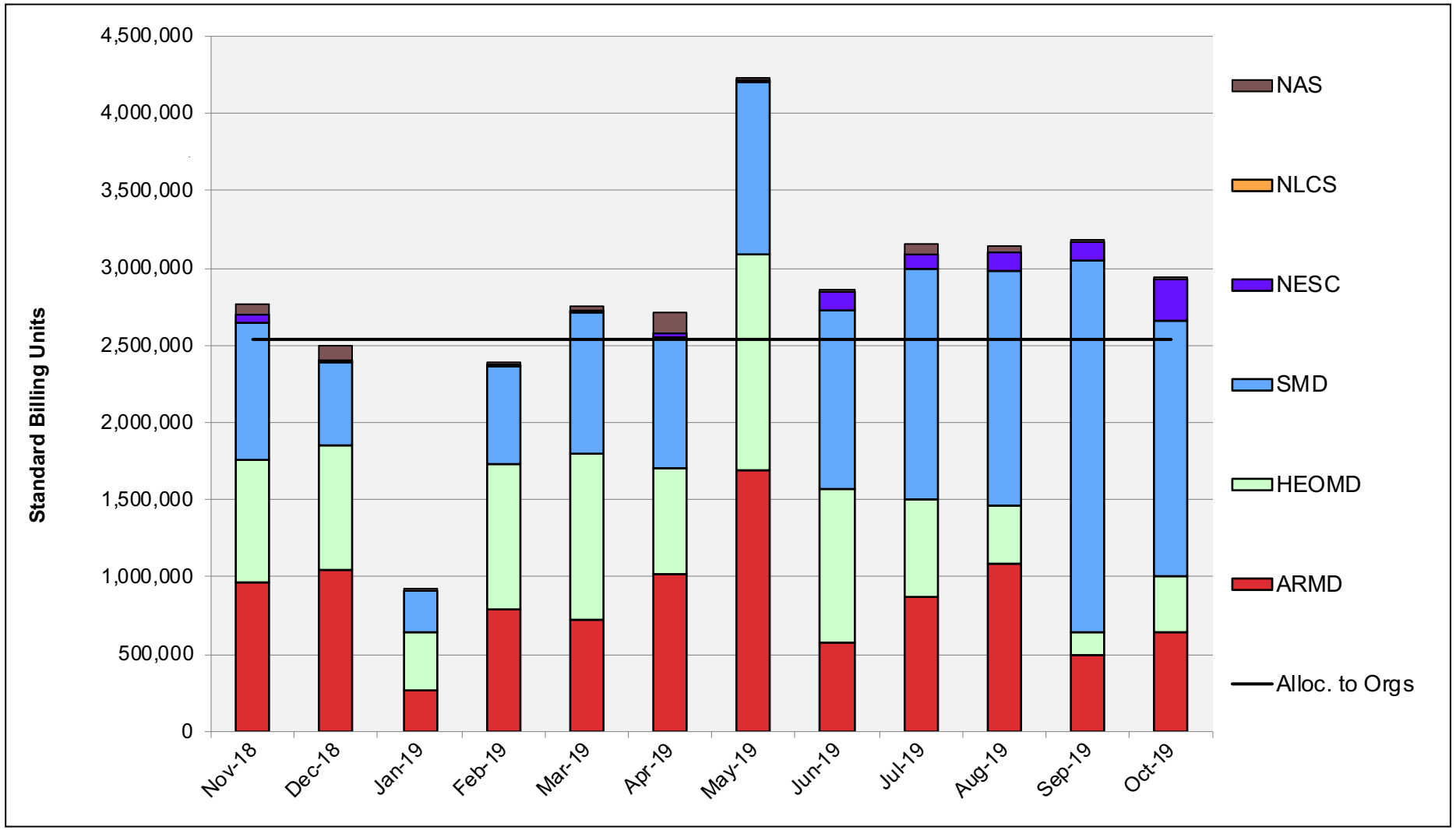
Aitken: Average Time to Clear All Jobs



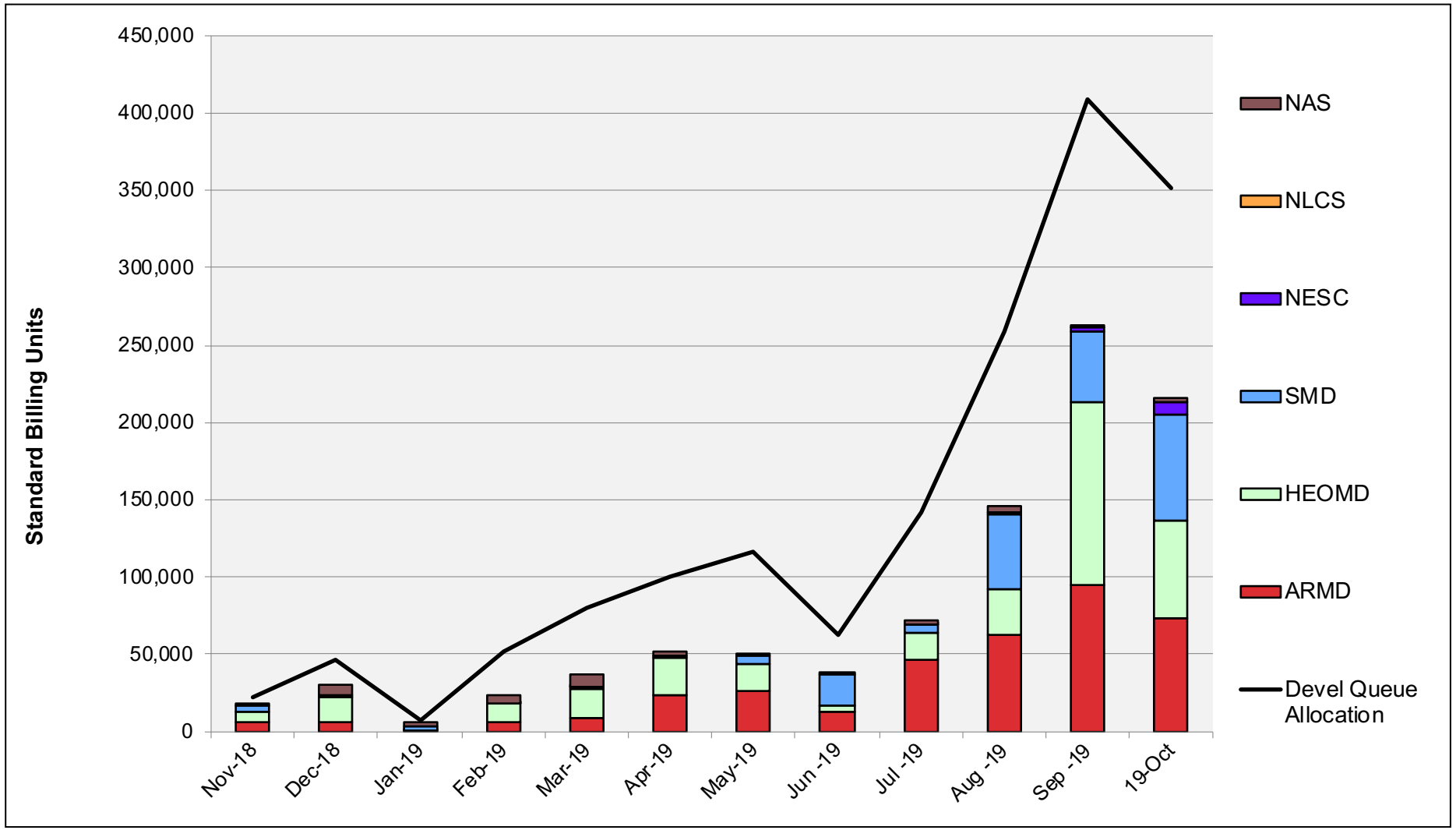
Aitken: Average Expansion Factor



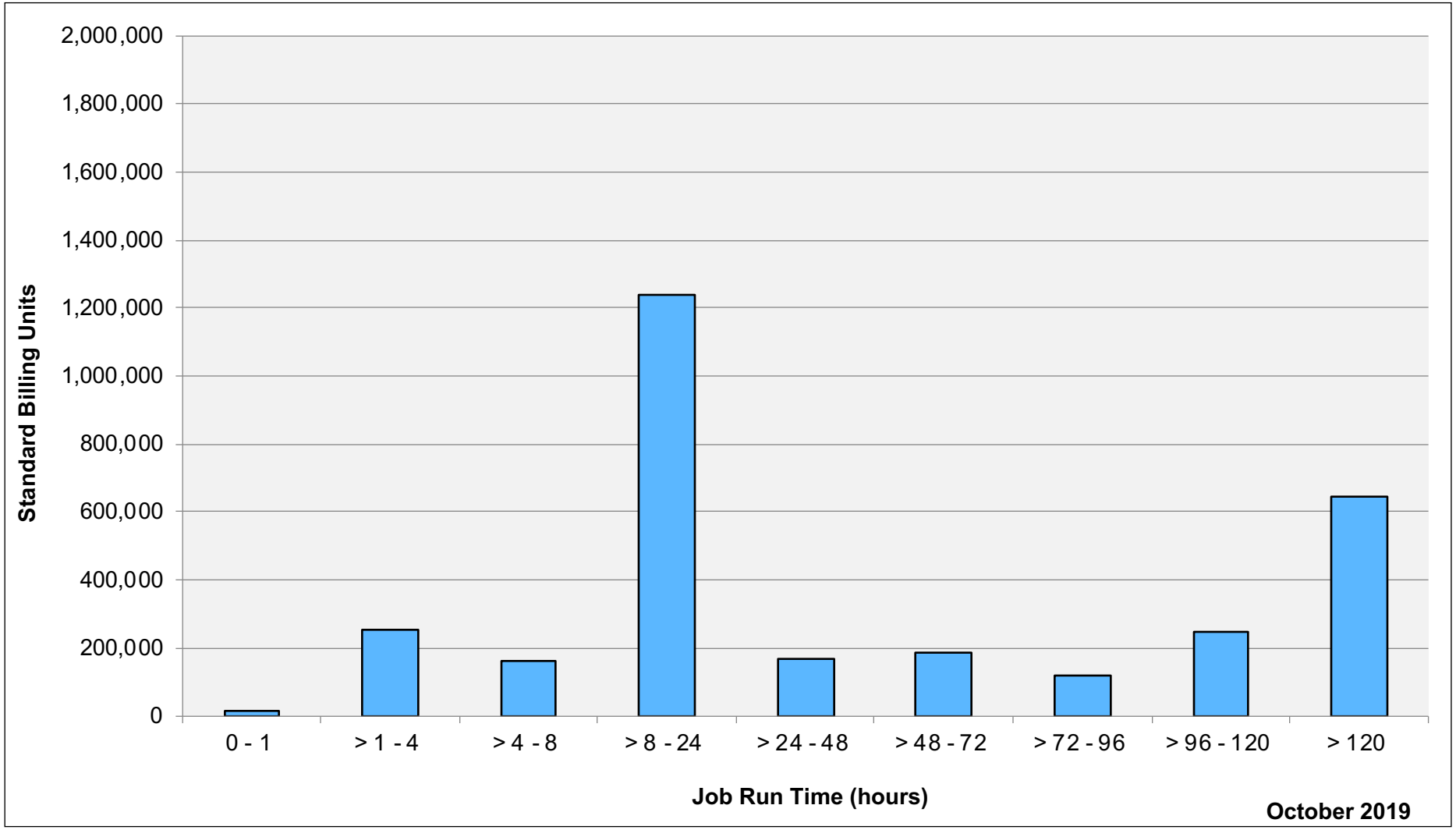
Electra: SBUs Reported, Normalized to 30-Day Month



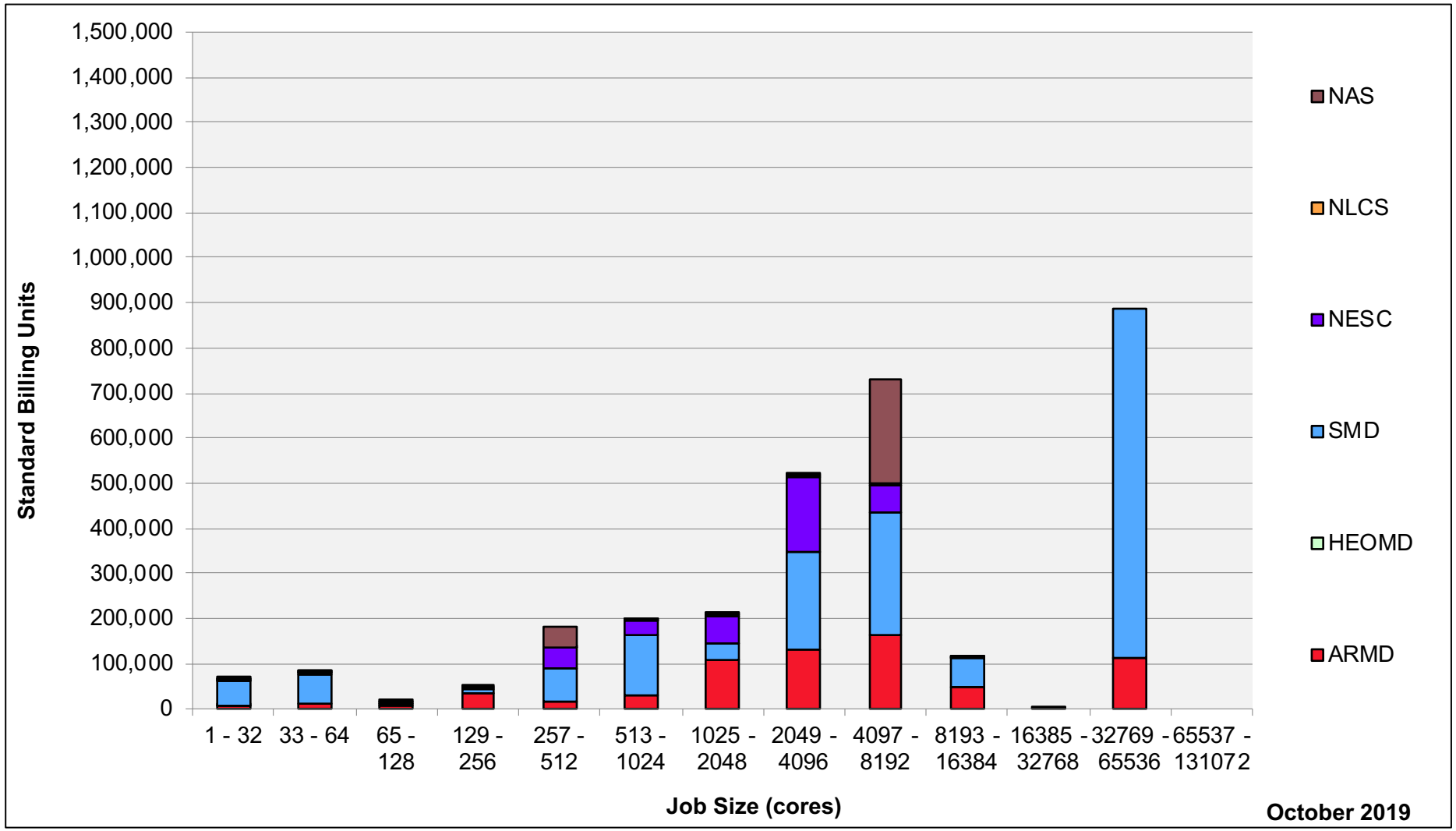
Electra: Devel Queue Utilization



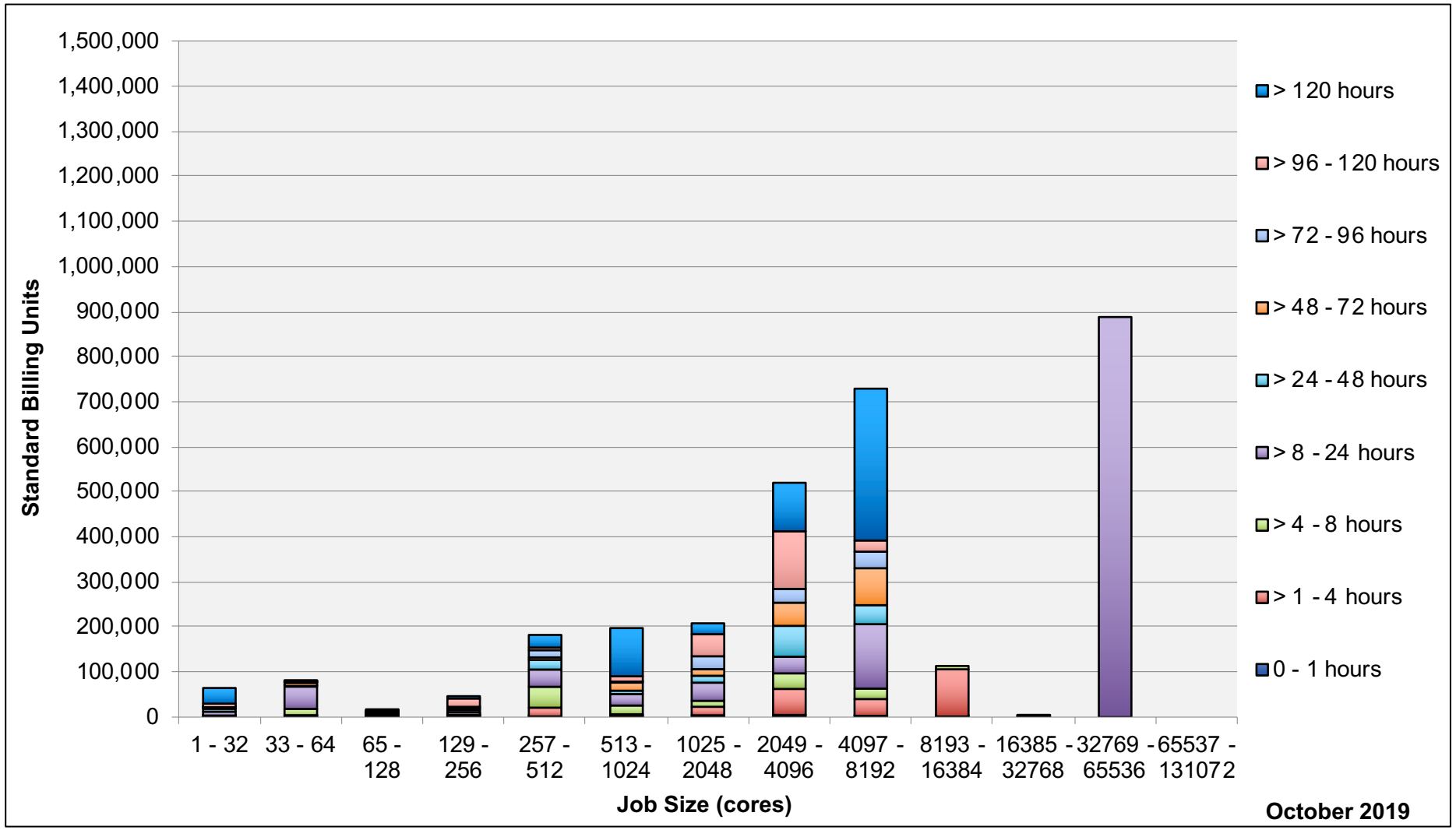
Electra: Monthly Utilization by Job Length



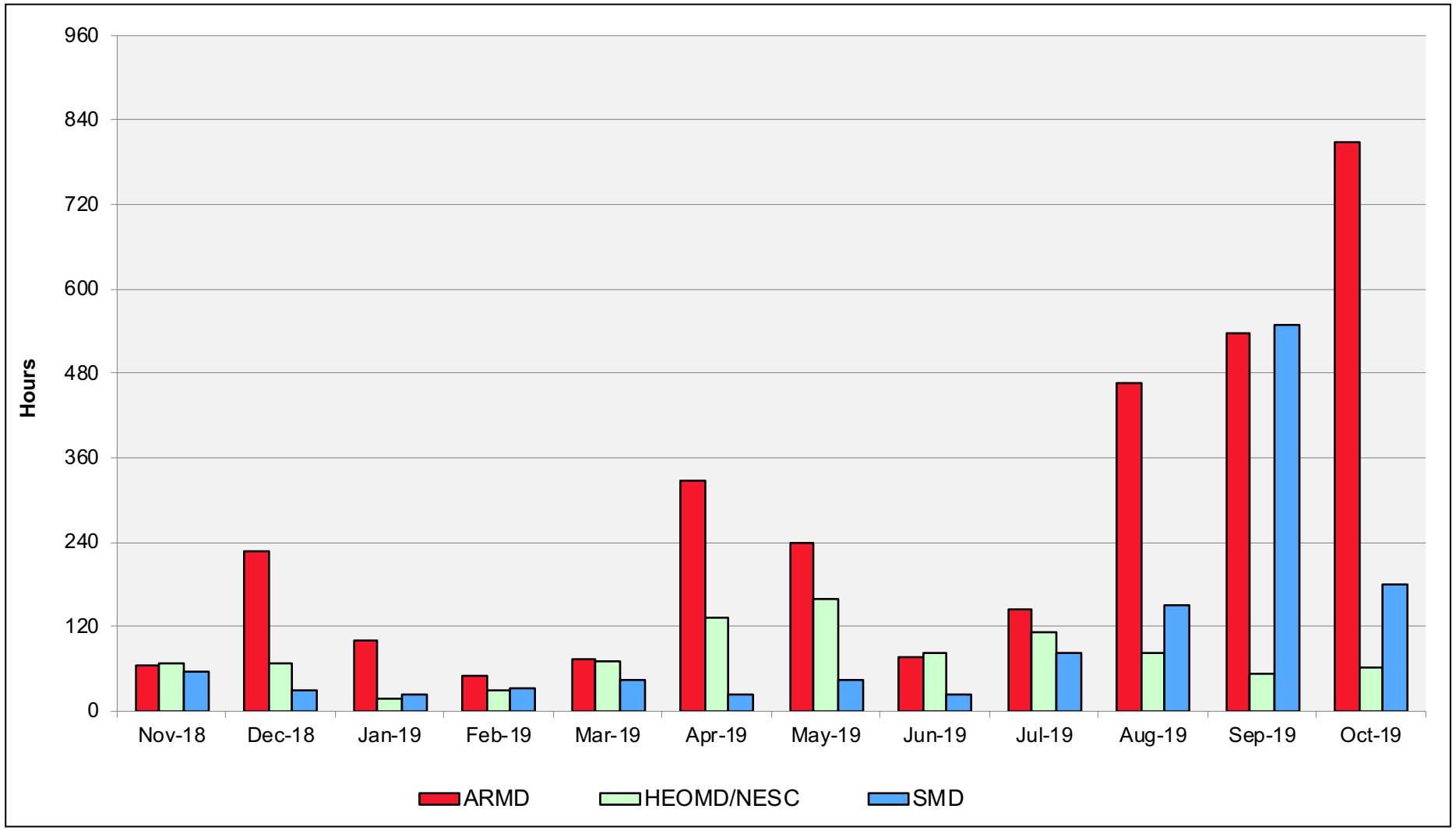
Electra: Monthly Utilization by Job Length



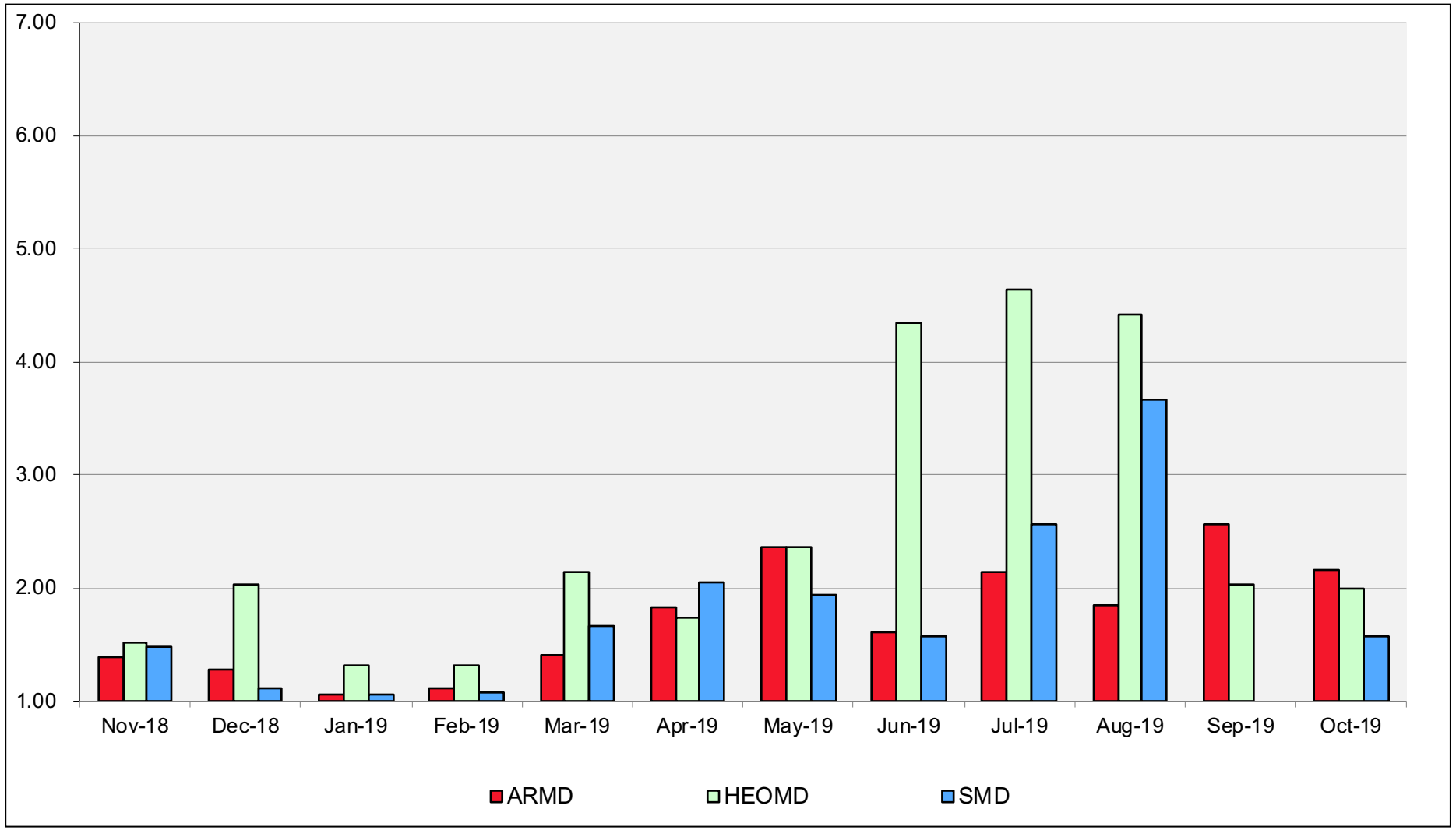
Electra: Monthly Utilization by Size and Length



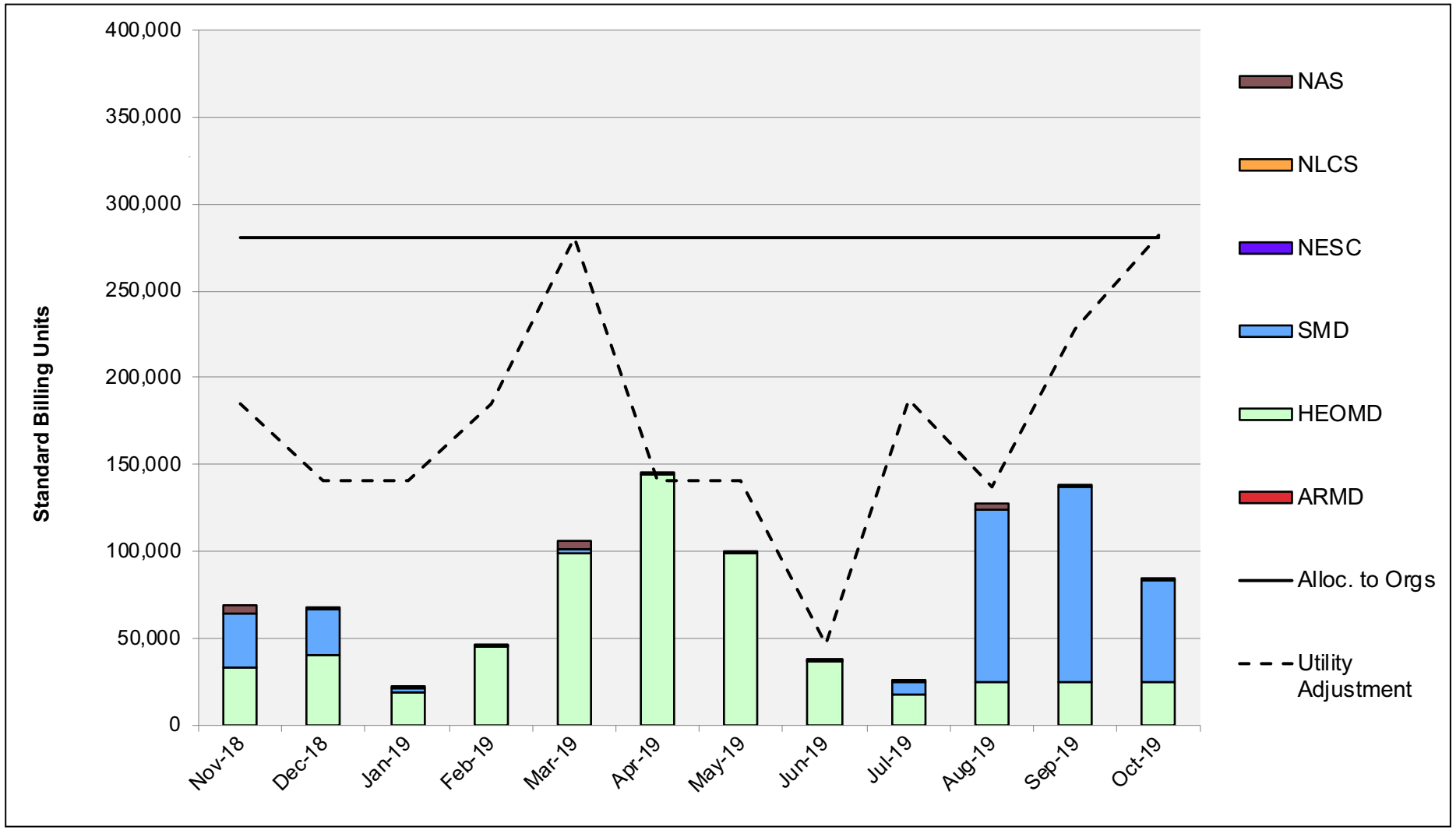
Electra: Average Time to Clear All Jobs



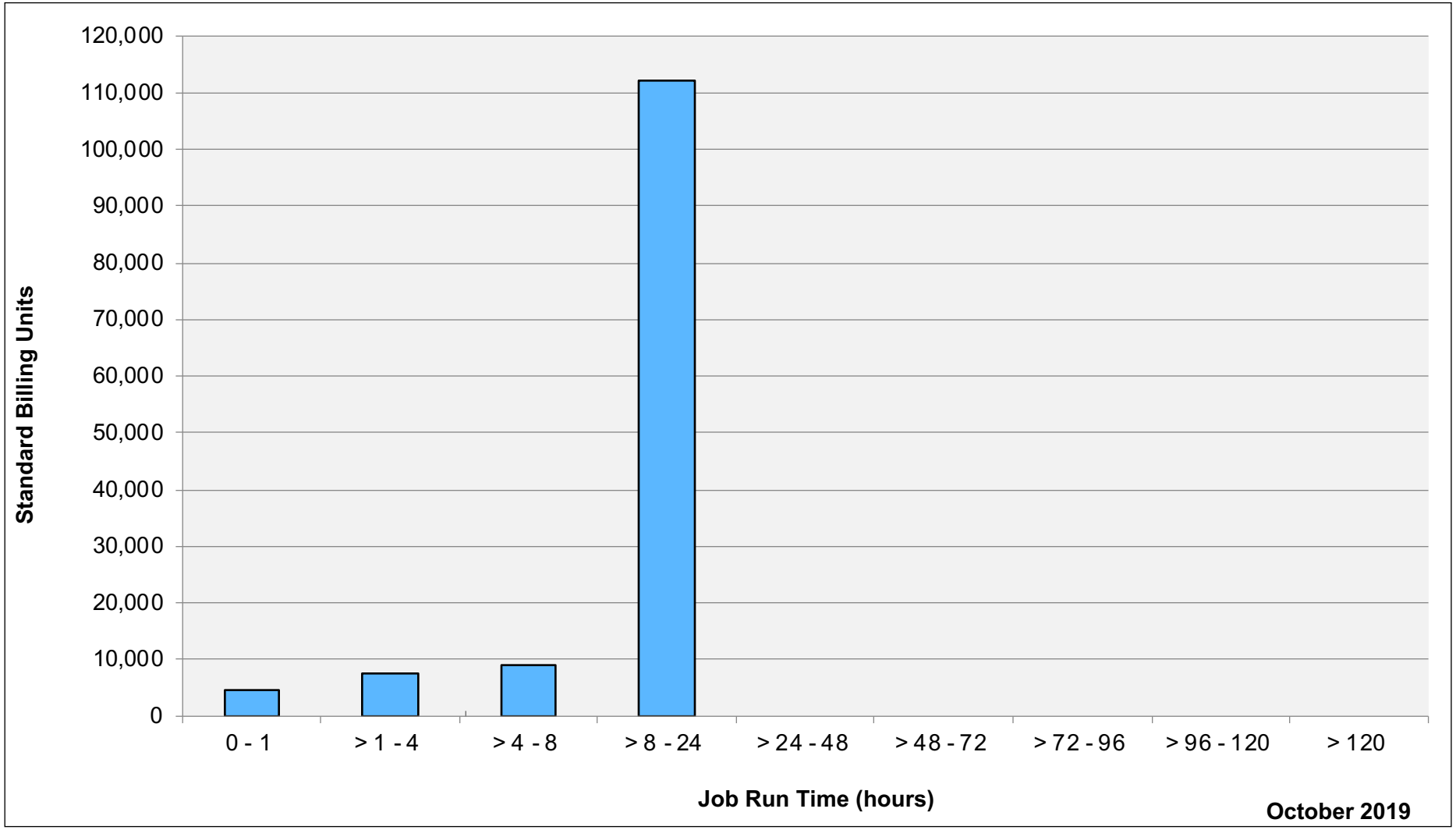
Electra: Average Expansion Factor



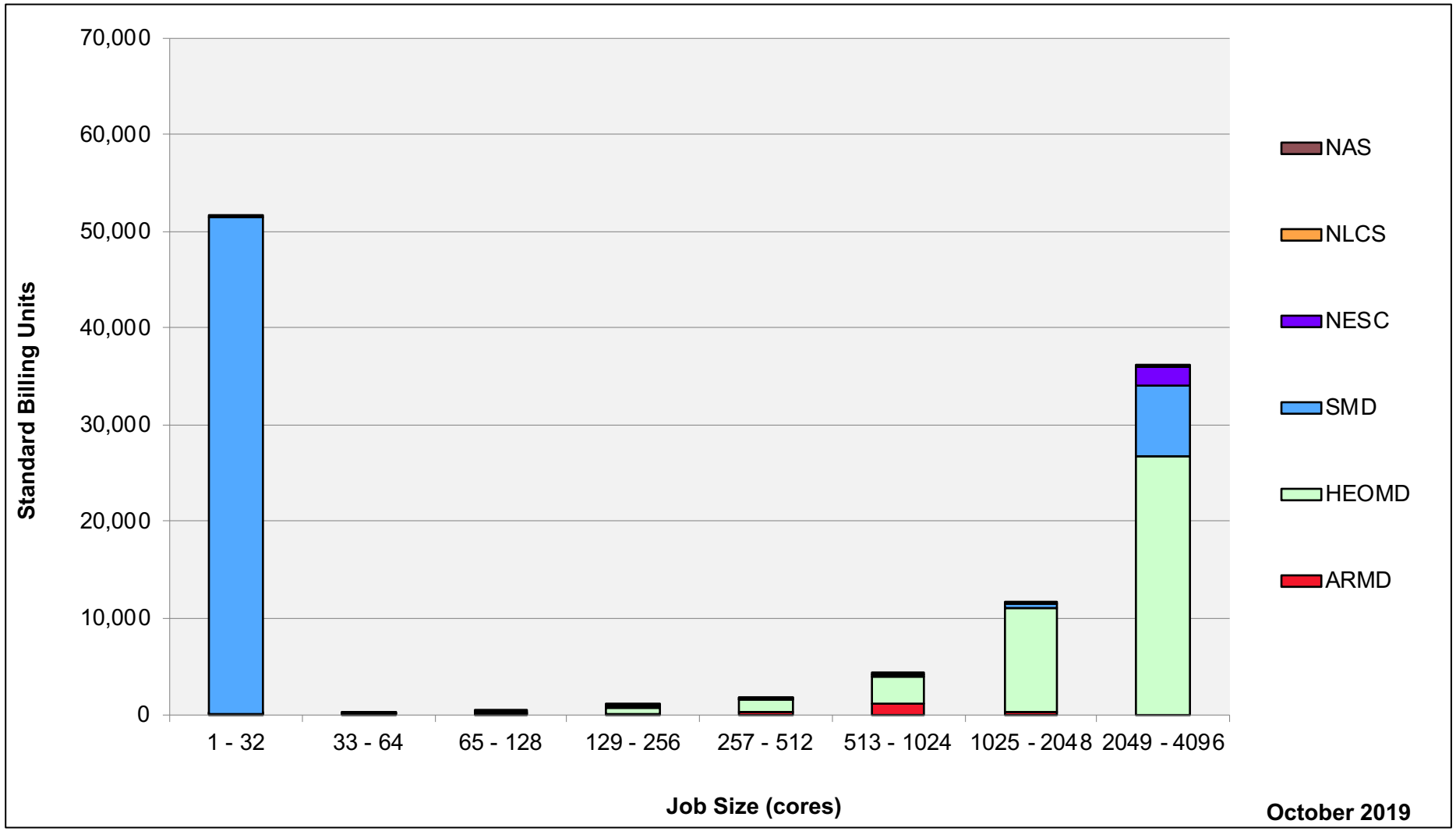
Merope: SBUs Reported, Normalized to 30-Day Month



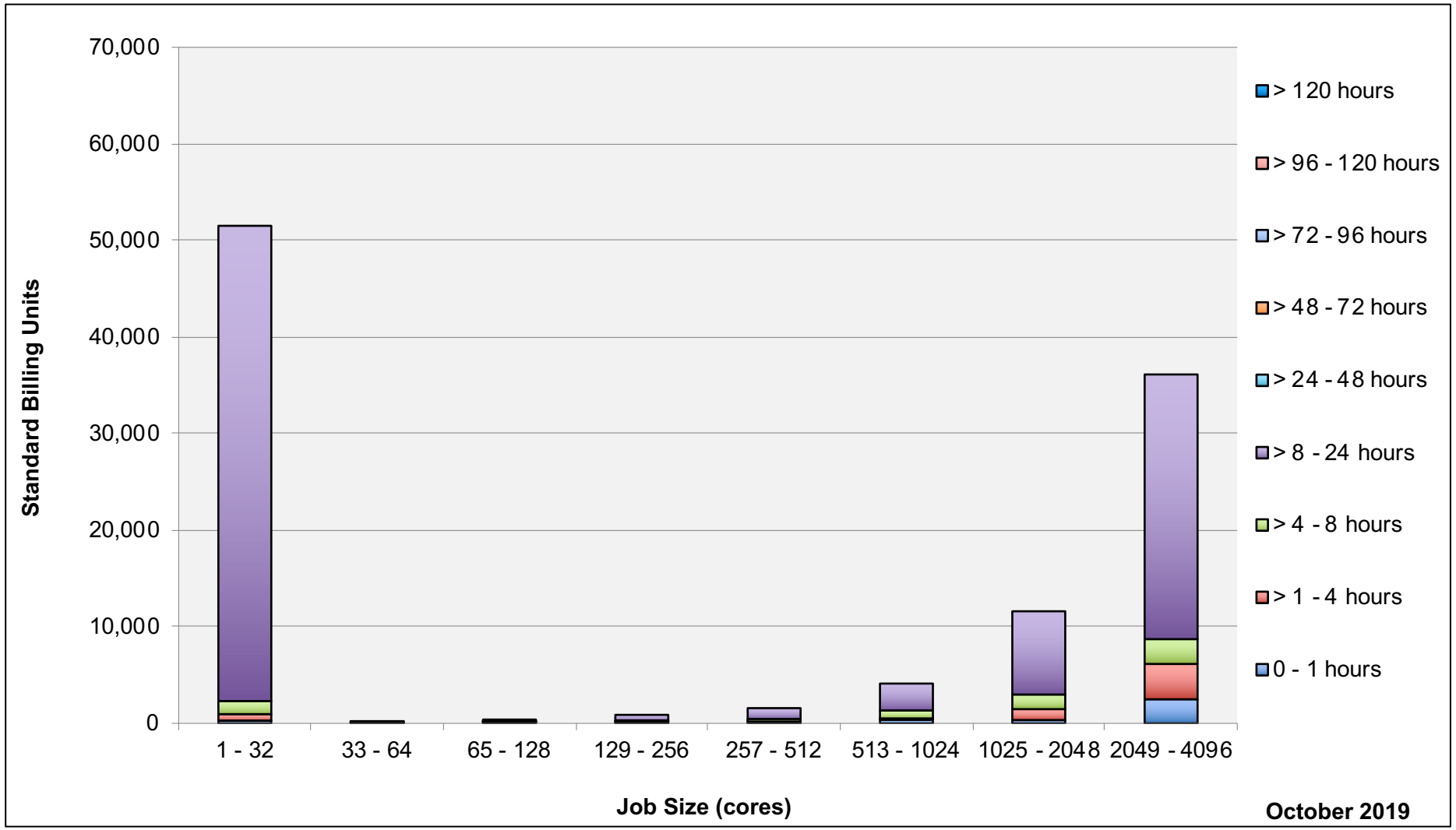
Merope: Monthly Utilization by Job Length



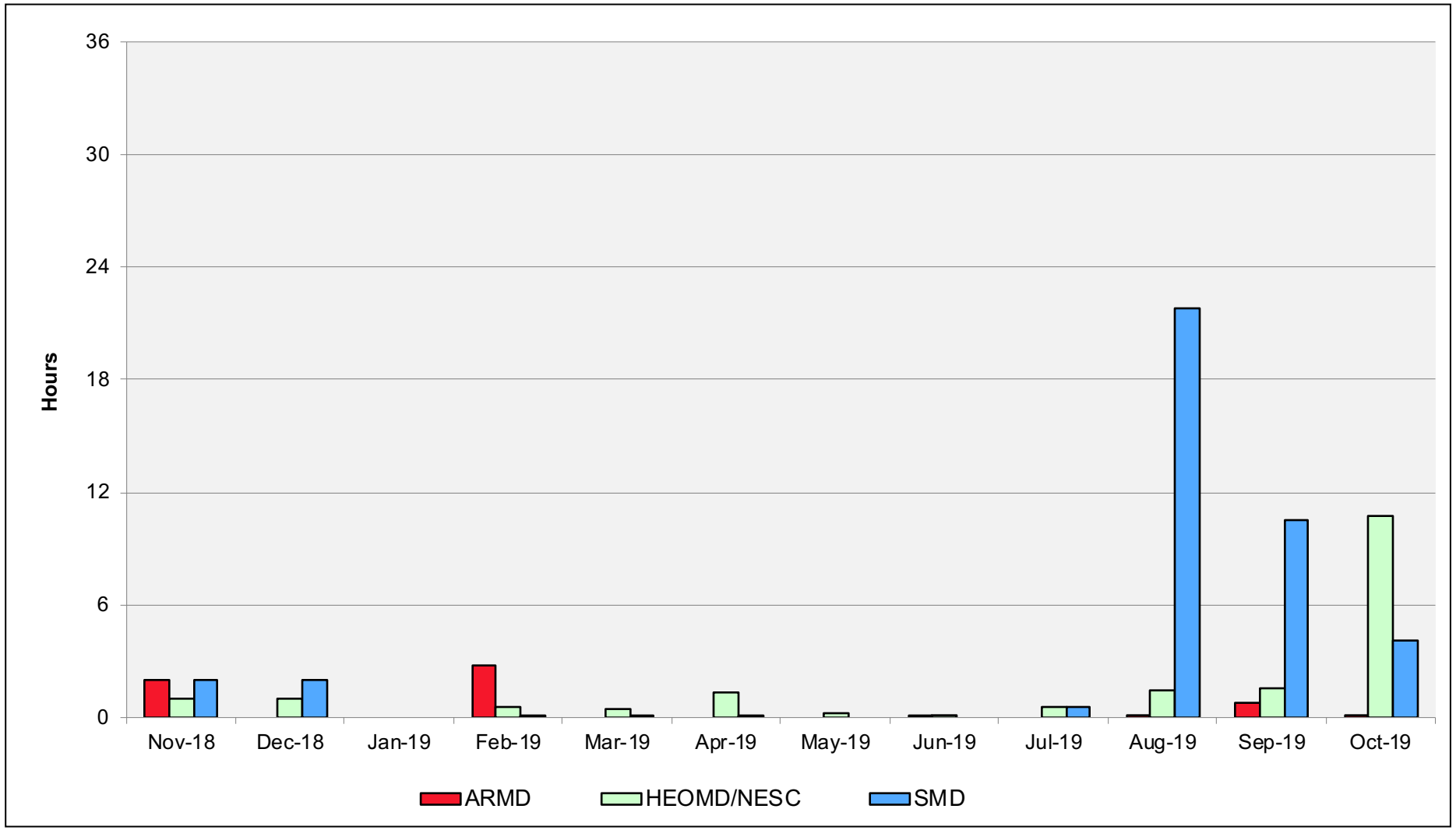
Merope: Monthly Utilization by Job Length



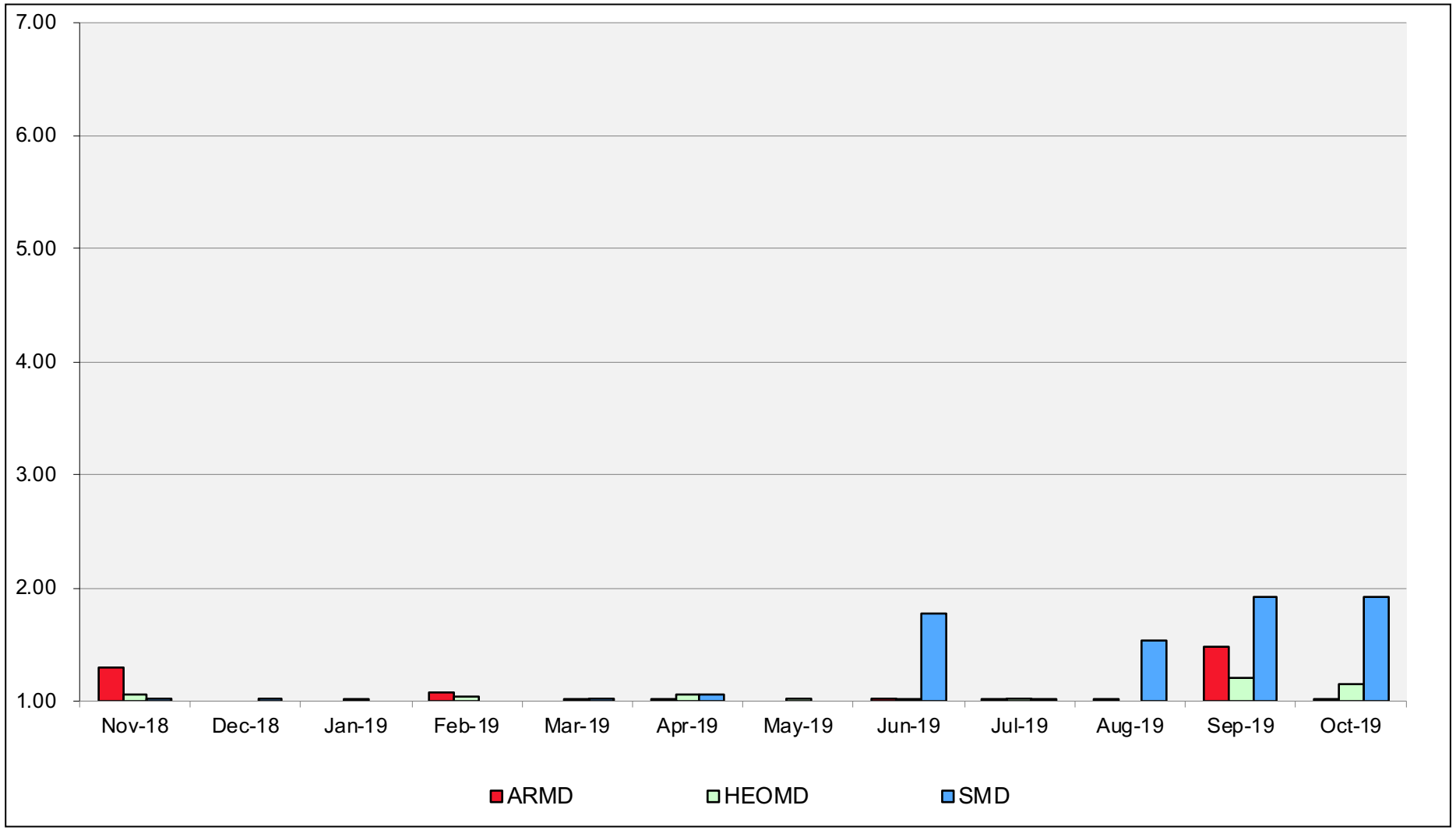
Merope: Monthly Utilization by Size and Length



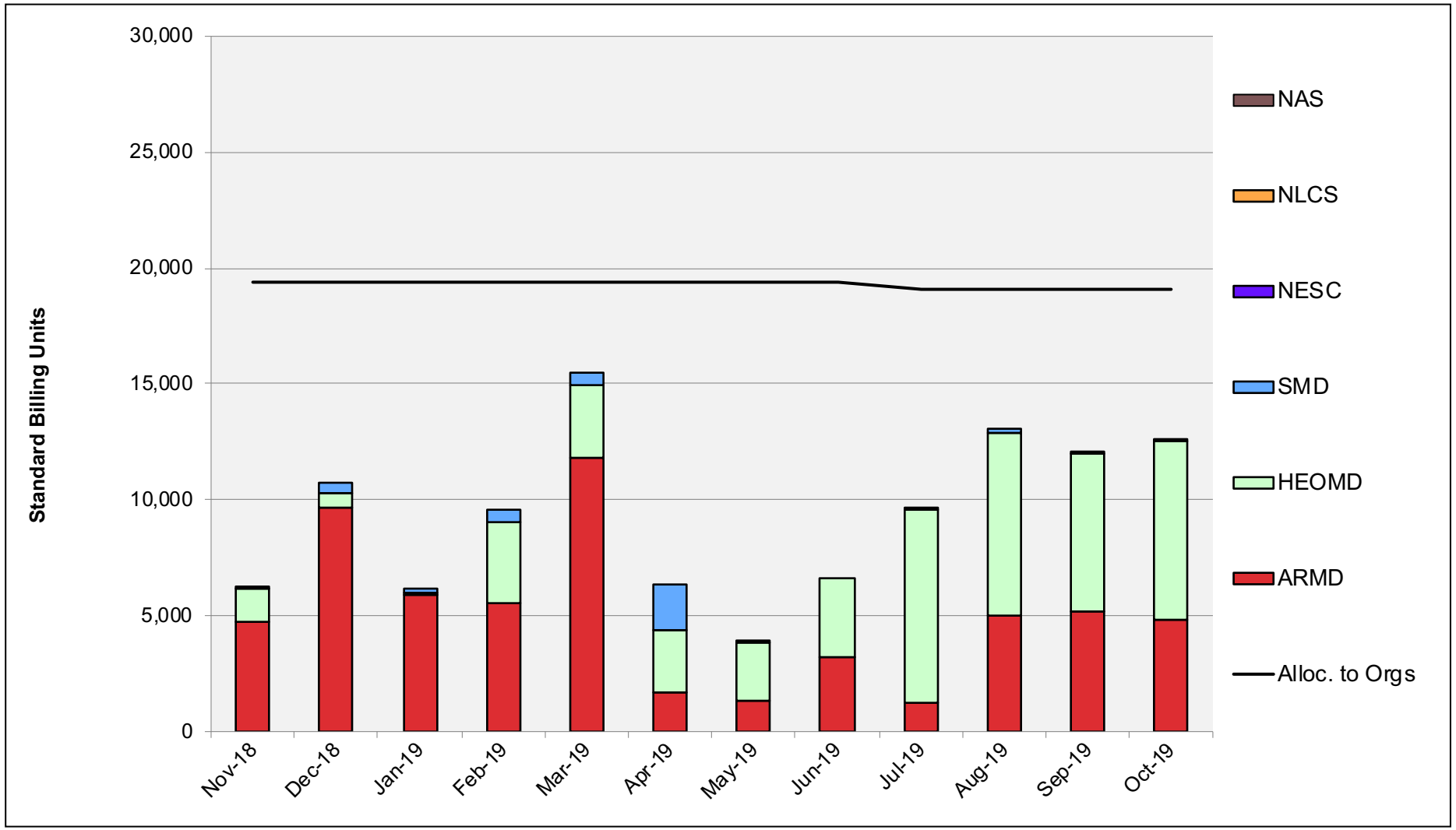
Merope: Average Time to Clear All Jobs



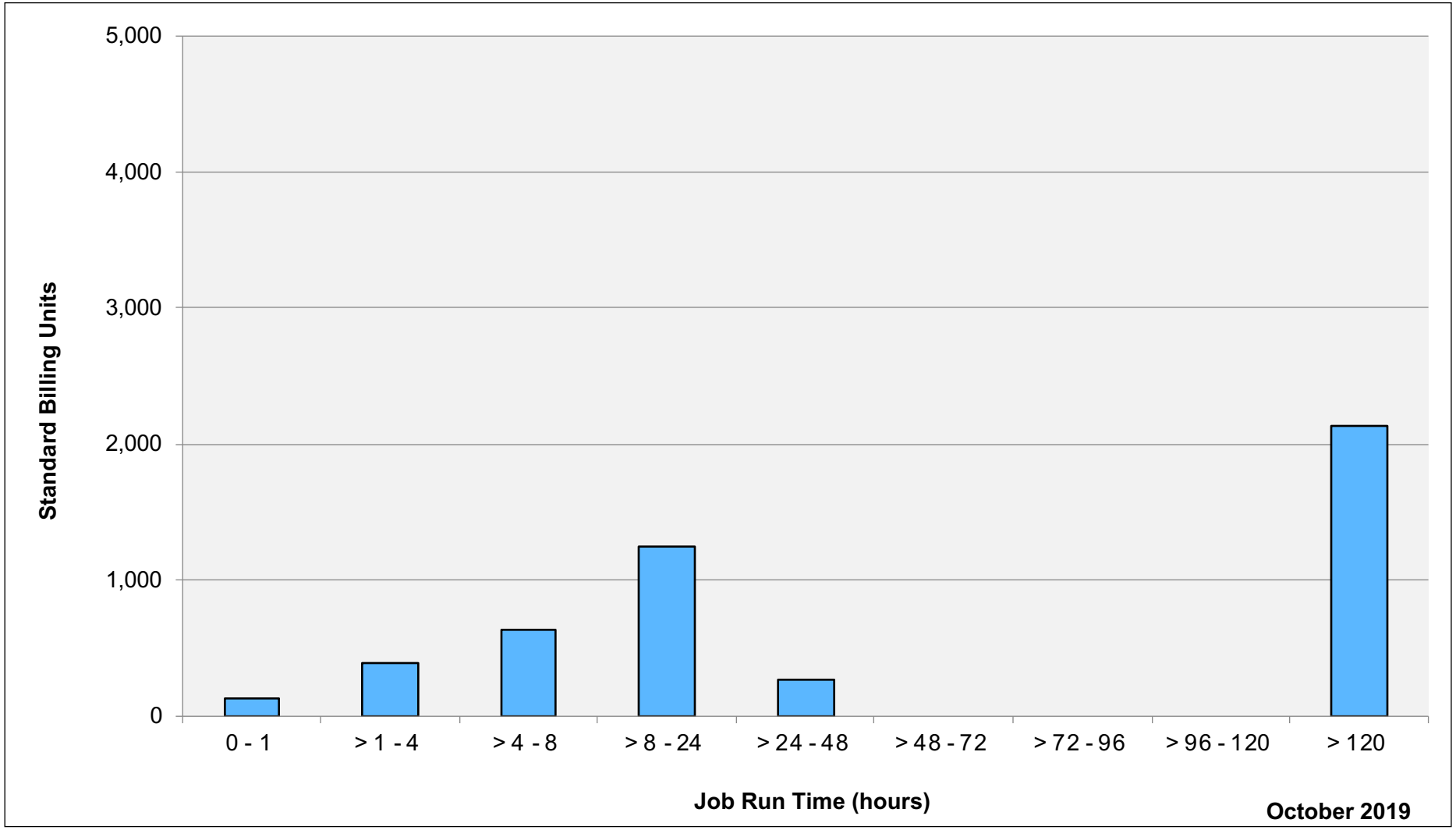
Merope: Average Expansion Factor



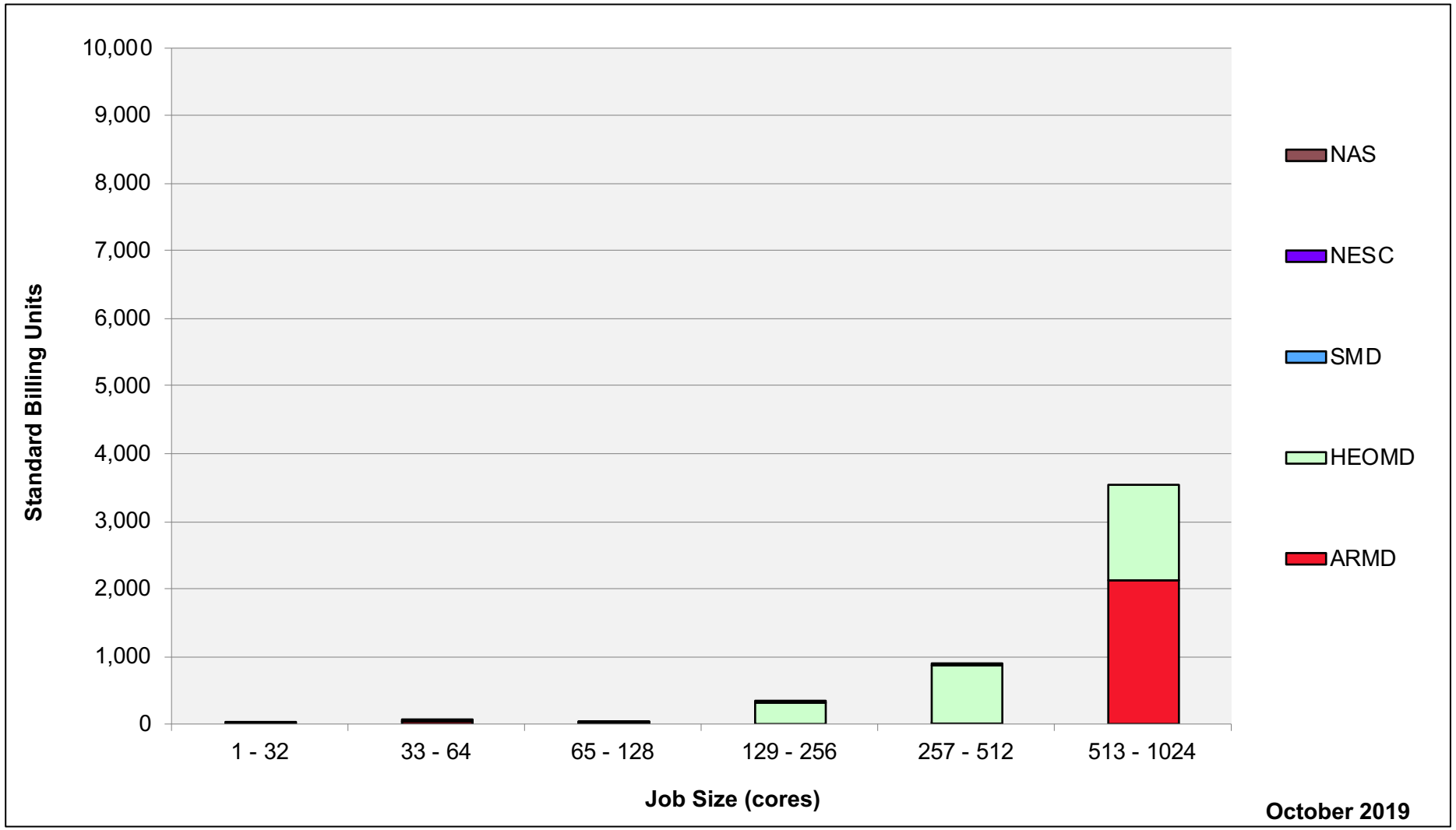
Endeavour: SBUs Reported, Normalized to 30-Day Month



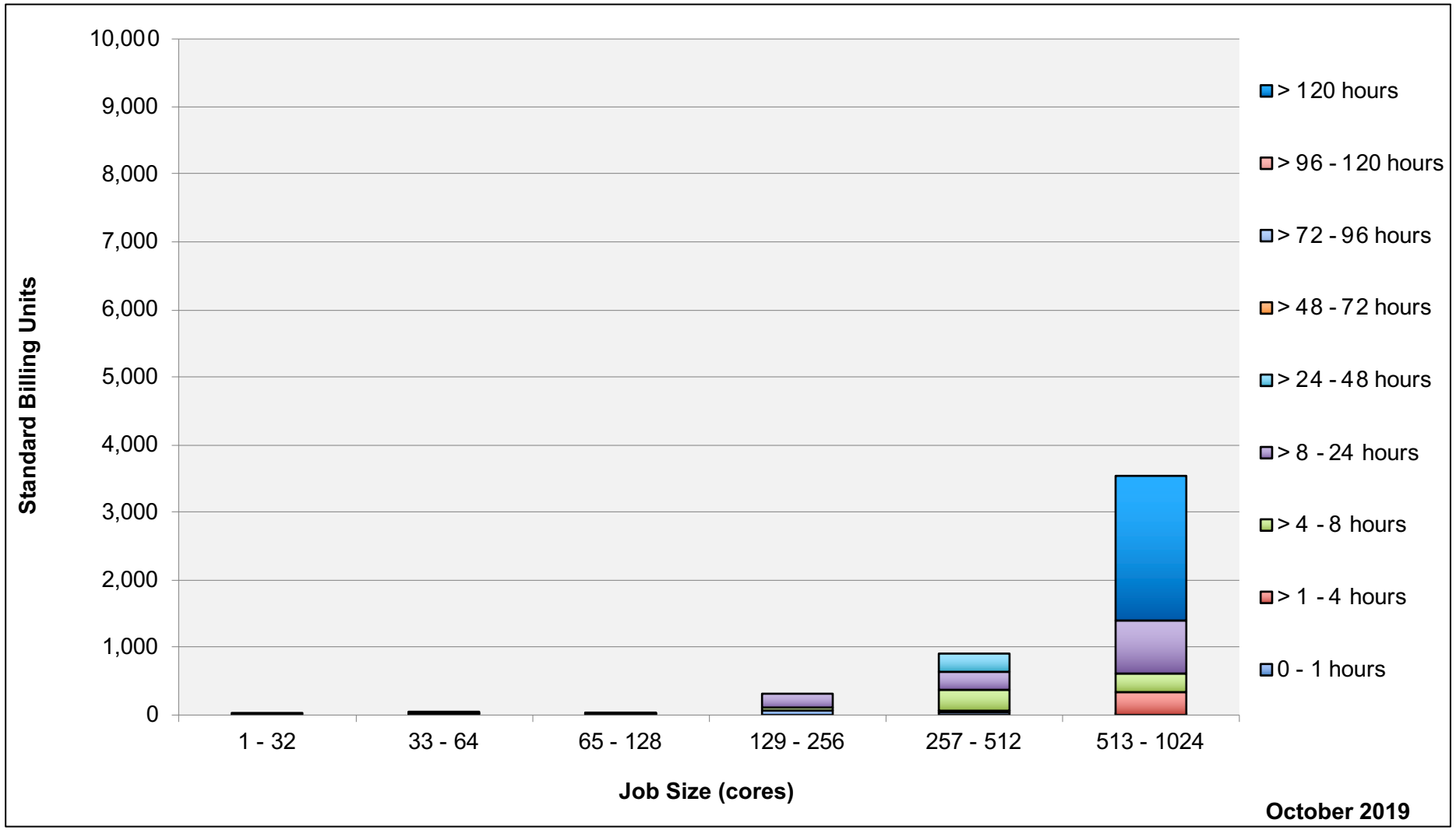
Endeavour: Monthly Utilization by Job Length



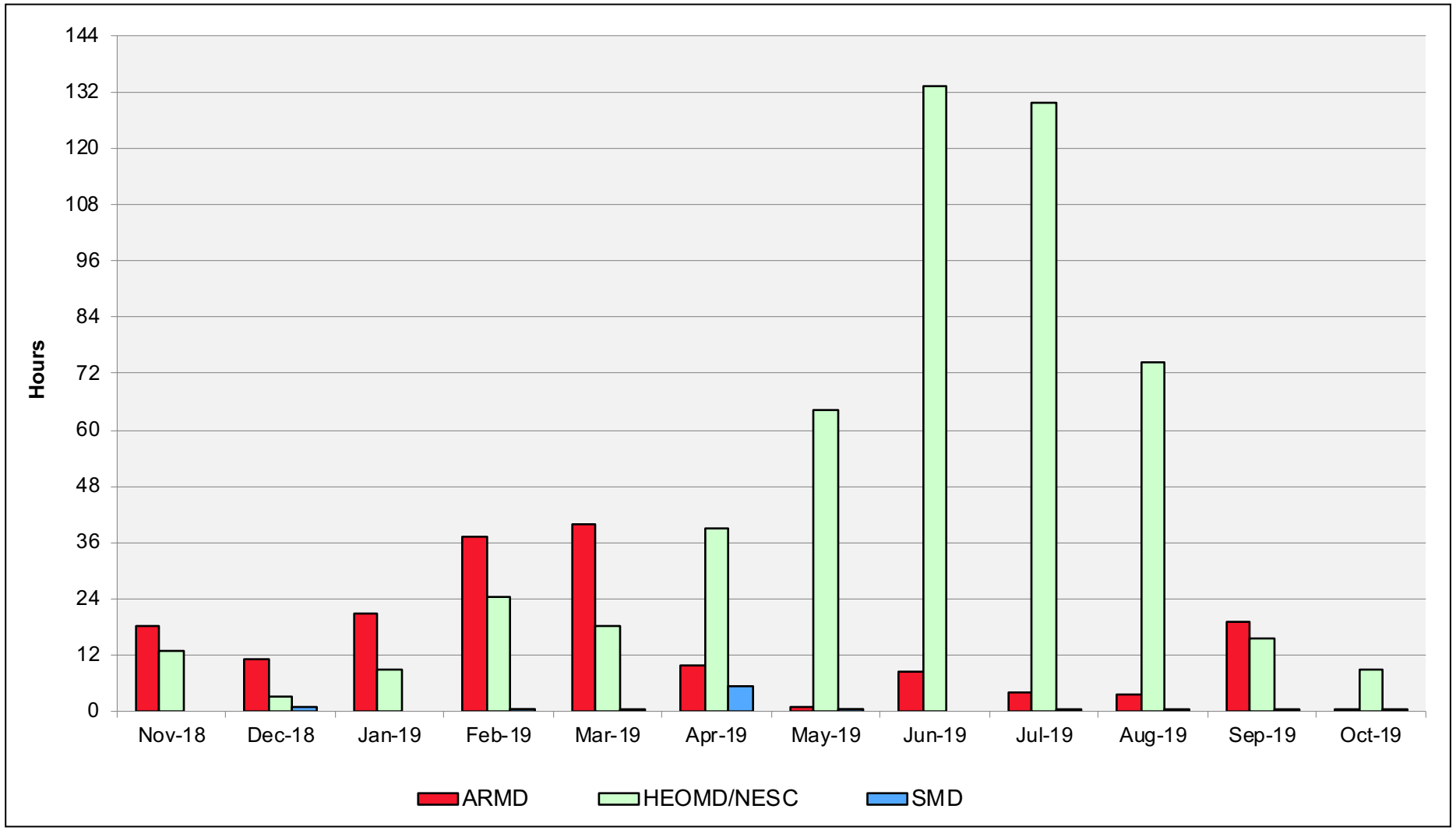
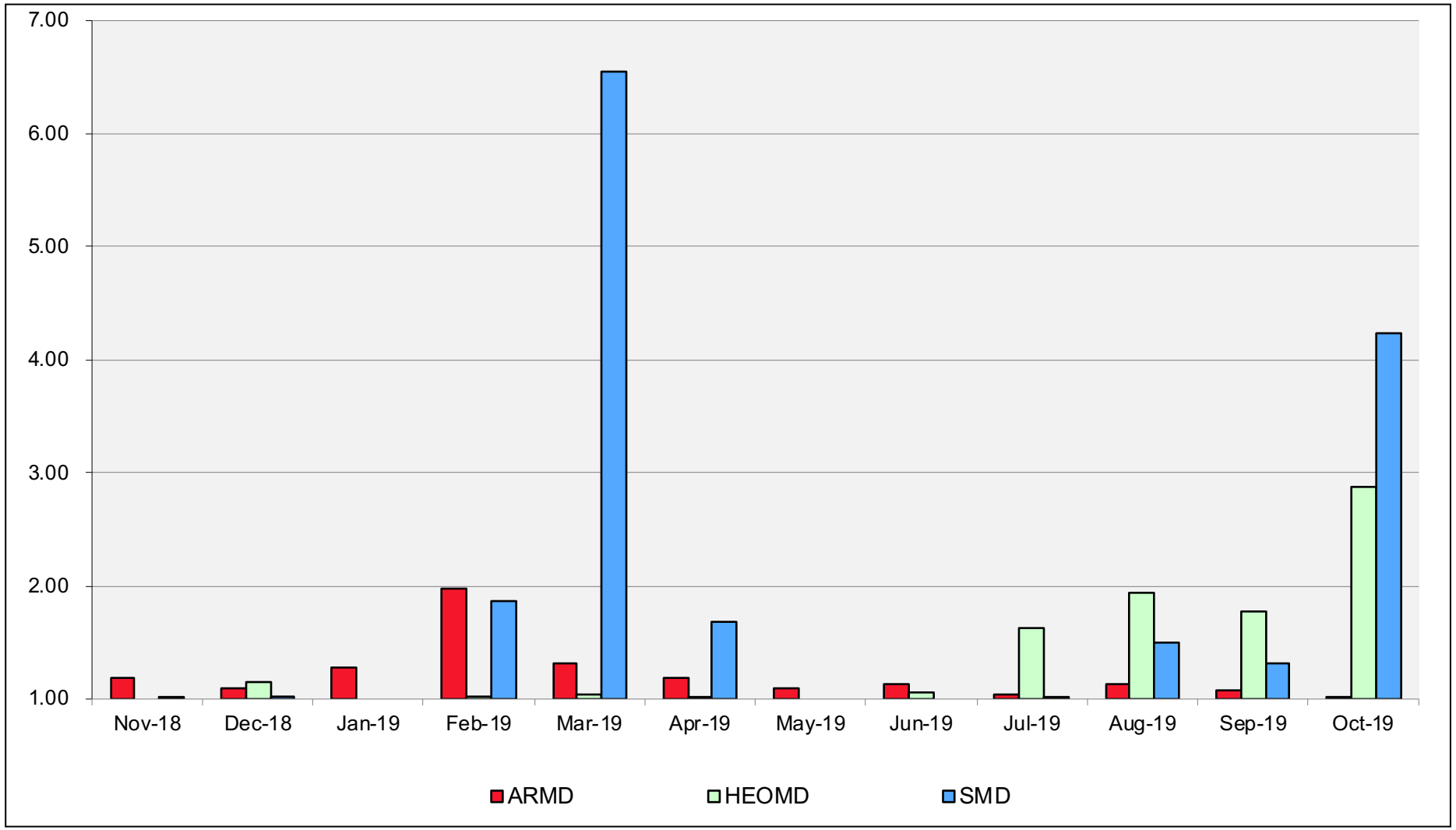
Endeavour: Monthly Utilization by Job Length



Endeavour: Monthly Utilization by Size and Length



Endeavour: Average Time to Clear All Jobs



Endeavour: Average Expansion Factor