National Aeronautics and
Space Administration

HIGH-END COMPUTING CAPABILITY PORTFOLIO

William Thigpen
NASA Advanced Supercomputing Division

October 10, 2019

Aitken Released to Users for Early Access Testing

- HECC released the recently installed new supercomputer, Aitken, for early-access users after extensive testing by staff.
- Aitken's four E-Cells provide 1,152 nodes with Intel Xeon Gold 5248 "Cascade Lake" processors, with a theoretical peak performance of 3.69 petaflops. The system's standard billing unit (SBU) rating was calculated at 1.64.*
- Like the previously deployed Electra supercomputer, Aitken is located in an energy-efficient modular facility that leverages the mild climate of the San Francisco Bay Area to achieve a highly efficient power utilization effectiveness (PUE) rating. Deployed in the first module of NASA's new Modular Supercomputing Facility (MSF), Aitken is expected to achieve a PUE of approximately 1.05.
- The initial configuration of Aitken has a maximum power usage of 650 kilowatts, but the installed module has a capacity of 2.5 megawatts and the full MSF site has a capacity of 30 megawatts to support future growth.

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

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

Aitken is deployed in the first module of NASA's Modular Supercomputing Facility, which is capable of holding an additional eight E-Cells before a second module is required.
David Ho, NASA/Ames

Successful Data Transfer & Processing During Wind Tunnel Test

- In support of the Space Launch System (SLS), HECC experts, in collaboration with engineers in the Ames Wind Tunnel Division, demonstrated the ability to securely transfer data directly from the 11-ft. Unitary Wind Tunnel to the NASA Advanced Supercomputing (NAS) facility, with complete data processing (see slide 5).
- This milestone concluded the third of a multi-phase collaboration, with the goal to provide near-real-time results of the wind tunnel experiments, viewable on the NAS hyperwall. This technology advance promises to increase the value of testing by:
  - Enabling an assessment of the data quality in a timeframe that will allow corrective action before the test concludes.
  - Allowing the test team to up-prioritize specific test conditions based on what was seen.
  - Reducing design cycle times by getting the results to the program engineers promptly at the conclusion of the test.
- The demonstration of successful near-real-time transfer and processing of data provides opportunities for future collaboration and research into more secure, uni-directional, robust, high bandwidth data transfer mechanisms.

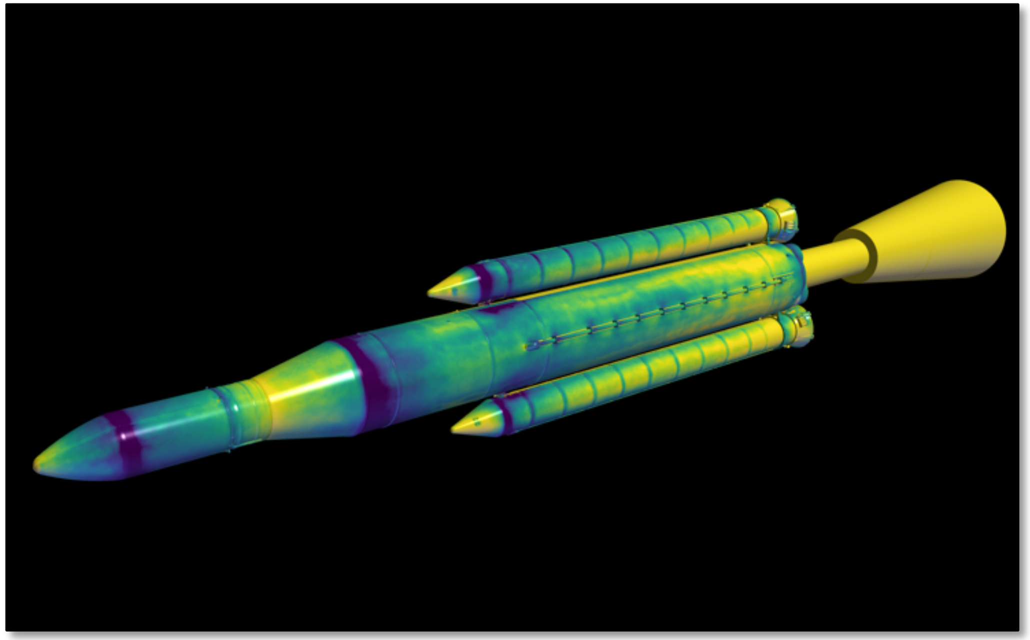
IMPACT: The direct, uni-directional connection from the Unitary Wind Tunnel to HECC supercomputers significantly reduced data transfer and processing turnaround time from months to minutes.

A secure, high-speed, uni-directional data transfer system allows data from cameras in the Ames Unitary Wind Tunnel to be sent directly to HECC supercomputers for immediate processing. *NASA/Ames*

Near-real-time Processing of Unitary Wind Tunnel Data on the Ames hyperwall

- HECC Visualization team provided significant, custom support for the live data transfer from the SLS transonic buffet test in the NASA Ames 11-ft Unitary Wind Tunnel (see slide 4), for near-real-time processing and display on the hyperwall—reducing customer access time from months to minutes.
- The 2.5% SLS model is covered with pressure sensitive paint, and the raw data are images showing its response over 5–10 seconds, at 10,000 frames per second, from each of four cameras. During a week of testing, such exposures at 800 test conditions produced about 160 terabytes data.
- The primary data processing used computer vision techniques to convert 2D pixel intensities into pressure values on the surface of the 3D model. The Visualization group reduced this processing time from one day per test point to one minute, using massive parallelism on HECC supercomputers.
- The near-real-time availability of results provides unprecedented opportunities to confirm data quality and to detect unforeseen behavior—while the test is still running in the wind tunnel—allowing corrective action and guiding further data acquisition.

IMPACT: Coupling Ames wind tunnels with Ames HECC supercomputers enables near-real-time data analysis, giving customers opportunities for timely corrections, data-guided exploration, and more efficient use of these expensive test facilities.



Visualization showing averaged pressure distribution on the surface of a model of the SLS in the NASA Ames 11-ft Unitary Wind Tunnel, as revealed by inline analysis of unsteady pressure sensitive paint streaming image data. *Chris Henze, NASA/Ames*

New Chillers Improve Availability of Merope

- Two new chillers were installed at the secondary NAS facility site (Building N233A) to provide cooling for the Merope supercomputer.
  - Each new chiller provides 90 tons of cooling. Bldg. N233A also has two existing chillers of 90 tons each. The new chillers replace two existing chillers that failed.
  - With all four chillers operating, N233A has a nominal cooling capacity of 360 tons, which is good for cooling 1.27 megawatts of power consumed by the computer equipment. Merope's maximum power draw is only 725 kilowatts.
- With the installation of the new chillers, the N233A cooling system has returned to full capacity, enabling all Merope nodes to be put into service.
  - Merope's compute capacity was temporarily reduced due to to the loss of cooling capacity when two existing chillers failed. After the chiller failures, temporary chillers were connected the N233A cooling system to allow Merope to continue to operate for three months.
  - Once the two new chillers started to provide chilled water to N233A, the temporary chillers were removed.
- The cooling system is now more robust with the new chillers and will improve Merope's availability to the HECC user community.

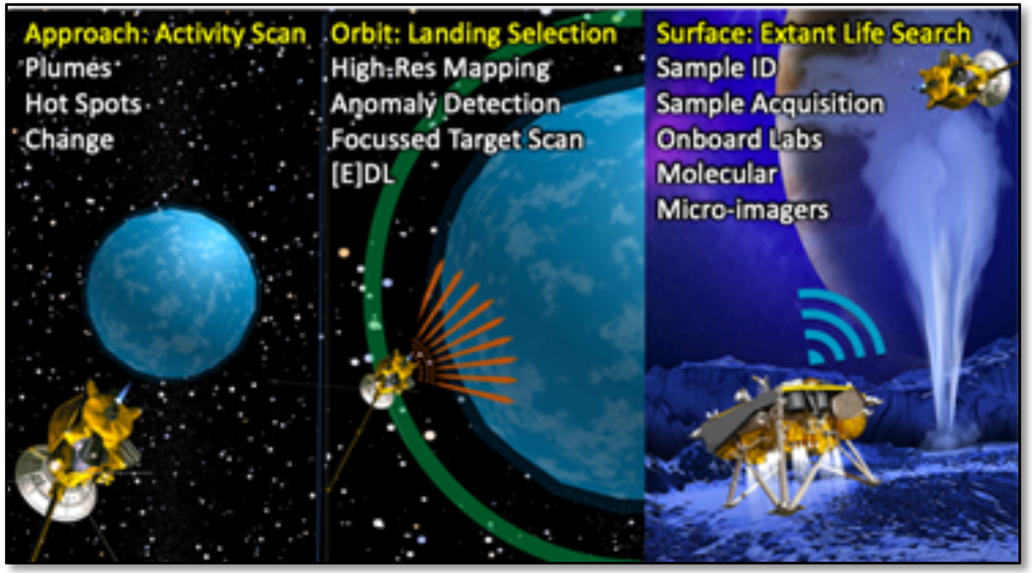
IMPACT: Maintaining a robust cooling system is crucial to the continuous operation of HECC supercomputing capabilities for NASA users.

Two new 90-ton chillers installed on the equipment pad at Building N233A at NASA Ames provide chilled water to the Merope supercomputer. *Chris Tanner, NASA/Ames*

Defining a New Paradigm for Space-borne Computing

- A member of the Applications Performance and Productivity (APP) team participated in the "Nebulae: Deep-Space Computing Clouds" workshop run by the Keck Institute for Space Studies.
- A group of about 25 people —mostly from JPL—is exploring ways to increase computing resources on space missions in order to lessen the reliance on downloading sensor data to Earth.
- The APP contribution centered around the specification of computing tasks and how they would be scheduled—in a manner similar to job scheduling on HECC systems.
- If the group's recommendations are adopted, there would be a new computing paradigm for NASA missions beyond low earth orbit: they would collect and archive large amounts of data onboard; users on Earth would use onboard computing to select and process the data of interest before downloading back to Earth.
- A follow-up workshop will be held in six months, with a goal of producing a white paper to use to gauge interest from potential funding sources.

IMPACT: Increasing the computing available to space missions will enable more mission autonomy and sophisticated science data services.



A "killer app" for the new space-borne architecture. With sufficient on-board computing power, a site selection mission can be combined with a lander mission, saving a significant amount of money. *Image courtesty of Keck Institute for Space Sciences Study Program: Nebulae: Deep-Space Computing Clouds.*

Preparing for the Future with OpenMP Code Hackathons

- Application Performance and Productivity (APP) staff participated as both a member and mentor in two code hackathons organized by National Energy Research Scientific Computing Center (NERSC) in Oakland and Berkeley. The goal of the hackathons is to speed up the porting process of OpenMP codes to modern architectures, such as GPUs.
  - A total of 18 teams participated.
  - Each team was assigned mentors with expertise in programming languages, compiler support, and profiling tools.
  - Targeted hardware included Intel KNL, Intel Skylake with Nvidia V100 GPUs, and IBM Power with V100 GPUs.
- Key achievements from teams in which APP members participated:
  - The High Flyer team assessed the effort to port legacy CFD codes to accelerators using OpenMP 4.5 directives, and achieved a 40% speedup using GPUs as compared to CPUs, which was found to be acceptable considering the short amount of development time.
  - The Michigan State University Center for Dynamical Systems team demonstrated the use of OpenMP to improve the memory efficiency for a beam-simulation framework.
- Lessons learned from these events will enable HECC to host future hackathons to further the goal of code modernization across more application teams.

IMPACT: HECC expertise helps ease the process of porting legacy codes to use accelerators, and will help ensure NASA’s effective use of future high-performance computing platforms.

The High Flyer Team at the NERSC Oakland Hackathon: CFD application experts come together with computer scientists and vendor engineers to port legacy codes to accelerators during the NERSC Oakland event held July 15–19, 2019. Third from right: HECC applications expert Gabriele Jost. *Photo courtesy David Eder, University of Hawaii*

JSC User Outreach Tour Aims to Improve Productivity

- In the second of three planned tours, a contingent of HECC staff visited users at Johnson Space Center (JSC) to highlight the project's extensive resources and services.
- The team held a successful discussion session with a small but very interactive group of scientists, engineers, and partners who depend on HECC resources and services for their NASA missions.
  - Users asked questions and received detailed information about the full range of services available to improve efficiency on HECC systems.
  - Attendees expressed a strong interest in how to set up jobs for parallel execution of numerous serial jobs. They were also interested in having more basic code optimization and best practices lessons.
  - Users were also interested in getting allocations for more compute resources. They suggested a center-funded seedling program to allow experimental codes to be tested before major allocation.
- The team will go to Marshall Space Flight Center in October to discuss similar opportunities and gather more information on users' needs.
- 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.

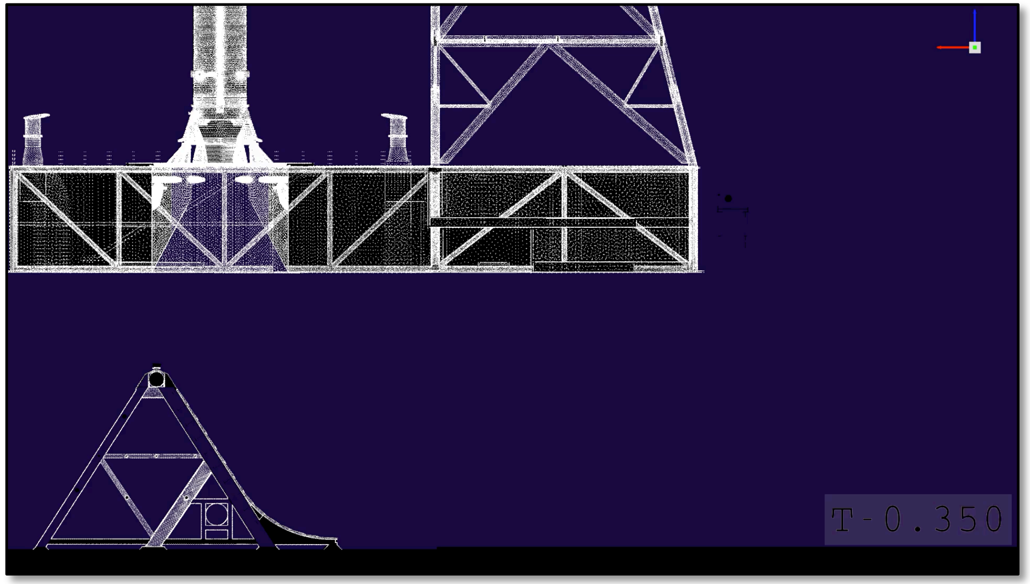
The restored Apollo 11 Mission Control Room at Johnson Space Center. *Blaise Hartman, NASA/Ames*

High-Resolution Launch Environment Simulations*

- CFD experts at NASA Ames applied high-resolution simulations methods to help identify thermal, pressure, and flow environments on and around the main flame deflector (MFD) at NASA Kennedy's Launch Complex 39B.
  – The KSC team stopped construction on the MFD, and requested Ames design analyses focusing on gaps between the MFD and the trench wall, and the gaps between the steel plates of the MFD, which could pose launch safety and maintenance concerns.
- The Ames team completed large-scale, high-end CFD simulations of highly detailed as-built pad geometry, which required them to develop appropriate boundary conditions, meshing, and lift-off information.
  – Simulations were performed with the Ames-developed LAVA code; post-processing was conducted using statistical tools from the LAVA framework.
  – Thermal environment simulations were conducted using LAVA's unstructured CFD code, utilizing a boundary layer resolved mesh and conjugate heat transfer within the MFD metal.
  – The simulations are some of the largest run on HECC systems—the LAVA Cartesian simulation contained over 555 million cells, over 500,000 timesteps.
- Data analysis and visualization were conducted by HECC visualization experts using custom in-house software.
- Results allowed MFD contractors to confidently continue the project, helped reduce mission risk, and saved significant amounts of time and money.

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

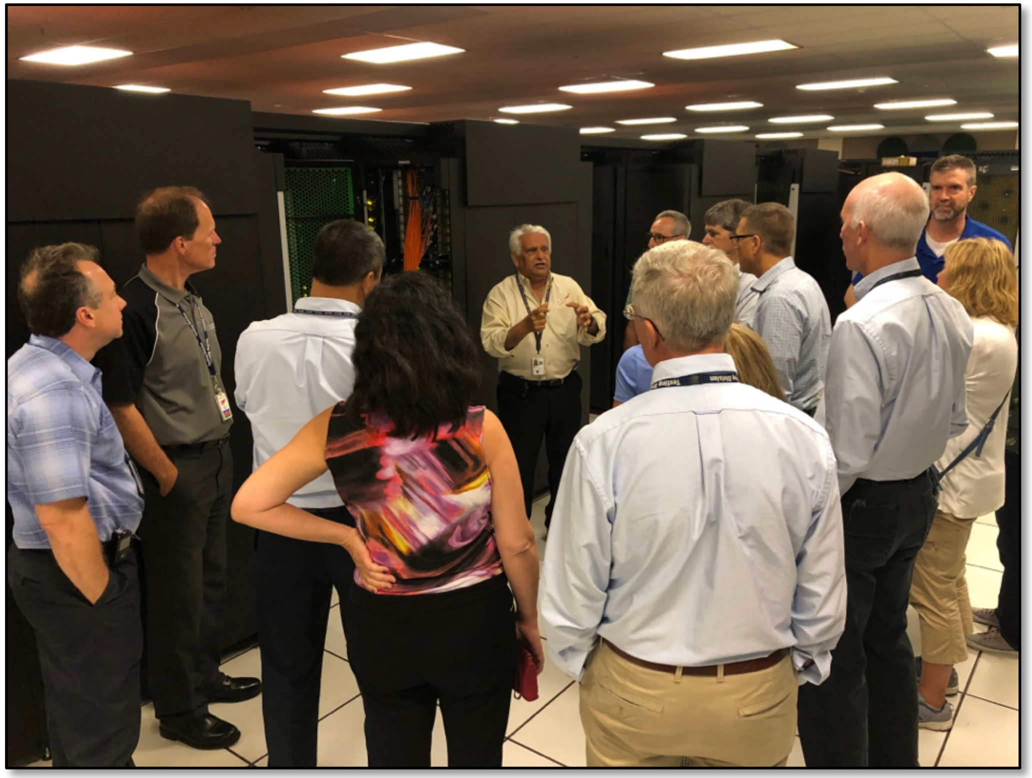
IMPACT: CFD simulation results guided NASA Kennedy project engineers in evaluating real-time design decisions for the main flame deflector redesign, and will help reduce mission risk.



Movie from a simulation of launch ignition for NASA's next-generation Space Launch System. Colors indicate temperature, where white is hotter and black is cooler. *Michael Barad, Tim Sandstrom, NASA/Ames*

HECC Facility Tours in September 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:
  - Clayton Turner, Deputy Center Director, Langley Research Center.
  - Gioia Deucher, CEO of Swissnex San Francisco.
  - The NASA High Resolution Imaging Experiment (HiRISE) Team.
  - Attendees of the Aerosciences Evaluation and Test Capabilities (AETC) Portfolio Face-to-Face Group meeting, who toured the NAS facility to promote possilbe future collaboration between aeronautics CFD simulation and wind tunnel testing.
  - Department of the Interior employees who visited the Ames Associate Director and Office of Safety and the Mission Assurance team.
  - A delegation from the National Supercomputing Centre Singapore, who were part of a Hewlett Packard Enterprise client visit.
  - A group from the Bay Area County Sheriff and Fire agency, who visited Ames for a site visit and evaluation of our high-value and high-risk assets.
  - Two groups from the Ames Fall Internship Program.



Piyush Mehrotra (back center), NASA Advanced Supercomputing (NAS) Division Chief, gives the Aerosciences Evaluation and Test Capabilities group a tour of the NAS supercomputer floor. *Gina Morello, NASA/Ames*

Papers

- **"A Decade of Variability on Jakobshavn Isbrae: Ocean Temperatures Pace Speed Through Influence on Mélange Rigidity**," I. Joughin, D. Shean, B. Smith, D. Floricioiu, The Cryosphere: Discussions, September 4, 2019. *
https://www.the-cryosphere-discuss.net/tc-2019-197/
- **"Optical Phase Curve of the Ultra-Hot Jupiter WASP-121b**," V. Bourrier, et al., arXiv:1909.03010 [astro-ph.EP], September 6, 2019. *
https://arxiv.org/abs/1909.03010
- "**TESS Observations of the WASP-121 b Phase Curve**," T. Daylan, et al., arXiv:1909.03000 [astro-ph.EP], September 6, 2019. *
https://arxiv.org/abs/1909.03000
- "**Shape and Size of Large-Scale Vortices: A Universal Fluid Pattern in Geophysical Fluid Dynamics**," L.-A. Couston, D. Lecoanet, B. Favier, M. Le Bars, arXiv:1909.03244 [physics.flu-dyn], September 7, 2019. *
https://arxiv.org/abs/1909.03244
- "**High-Frequency Plasma Waves and Pitch Angle Scattering Induced by Pulsed Electron Beams**," G. Delzanno, V. Roytershteyn, Journal of Geophysical Research: Space Physics, September 7, 2019. *
https://agupubs.onlinelibrary.wiley.com/doi/full/10.1029/2019JA027046
- **"Exact and Locally Implicit Source Term Solvers for Multifluid-Maxwell System**," L. Wang, A. Hakim, J. Ng, C. Dong, arXiv:1909.04125 [physics.comp-ph], September 9, 2019. *
https://arxiv.org/abs/1909.04125

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

Papers (cont.)

- "**Coronal Response to Magnetically-Suppressed CME Events in M-dwarf Stars**," J. Alvarado-Gómez, et al., arXiv1909.04042 [astro-ph.SR], September 9, 2019. *
  https://arxiv.org/abs/1909.04092
- "**Simulating Metal Mixing of Both Common and Rare Enrichment Sources in Low Mass Dwarf Galaxy**," A. Emerick, G. Bryan, M.-M. Mac Low, arXiv:1909.04695 [astro-ph.GA], September 10, 2019. *
  https://arxiv.org/abs/1909.04695
- "**dHybridR: a Hybrid—Particle-in-Cell Code Including Relativistic Ion Dynamics**," C. Haggerty, D. Caprioli, arXiv:1909.05255 [astro-ph.HE], September 11, 2019. *
  https://arxiv.org/abs/1909.05255
- **"Characterization of the L 98-59 Multi-Planetary System with HARPS**," R. Cloutier, et al., Astronomy & Astrophysics, vol. 629, September 13, 2019. *
  https://www.aanda.org/articles/aa/abs/2019/09/aa35957-19/aa35957-19.html
- "**Performance Optimization of Plate Airfoils for Martian Rotor Applications Using a Genetic Algorithm**," W. Koning, E. Romander, W. Johnson, presented at the European Rotorcraft Forum, Warsaw, Poland, September 17–20, 2019. *
  https://ntrs.nasa.gov/search.jsp?R=20190030870
- "**An Ideal Testbed for Planet-Disk Interaction: Two Giant Protoplanets in Resonance Shaping the PDS 70 Protoplanetary Disk**," J. Bae, et al., arXiv:1909.09476 [astro-ph.EP], September 20, 2019. *
  https://arxiv.org/abs/1909.09476

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

Papers (cont.)

- "**Conditional Generative Adversarial Networks (cGANs) for Near Real-Time Precipitation Estimation from Multispectral GOES-16 Satellite Imageries—PERSIANN-cGAN**," N. Hayatbini, et al., Remote Sensing, vol. 11, issue 19, September 20, 2019. *
https://www.mdpi.com/2072-4292/11/19/2193
- "**Three Red Suns in the Sky: A Transiting, Terrestrial Planet in a Triple M-dwarf System at 6.9 pc**," J. Winters, et al., The Astrophysical Journal, vol. 158, no. 4, September 23, 2019. *
https://iopscience.iop.org/article/10.3847/1538-3881/ab364d/meta
- "**Effects of Side Chain Length on Ionic Aggregation and Dynamics in Polymer Single-Ion Conductors**," L. Abbott, J. Lawson, Macromolecules, published online September 26, 2019. *
https://pubs.acs.org/doi/abs/10.1021/acs.macromol.9b00415
- "**Radiation Heat Transfer in a Gas Slab with Properties Characteristics of a Jet Engine Combustor**," A. Maurente, C. Alves, International Journal of Heat Mass Transfer, vol. 145, published online September 27, 2019. *
https://www.sciencedirect.com/science/article/pii/S0017931019328303

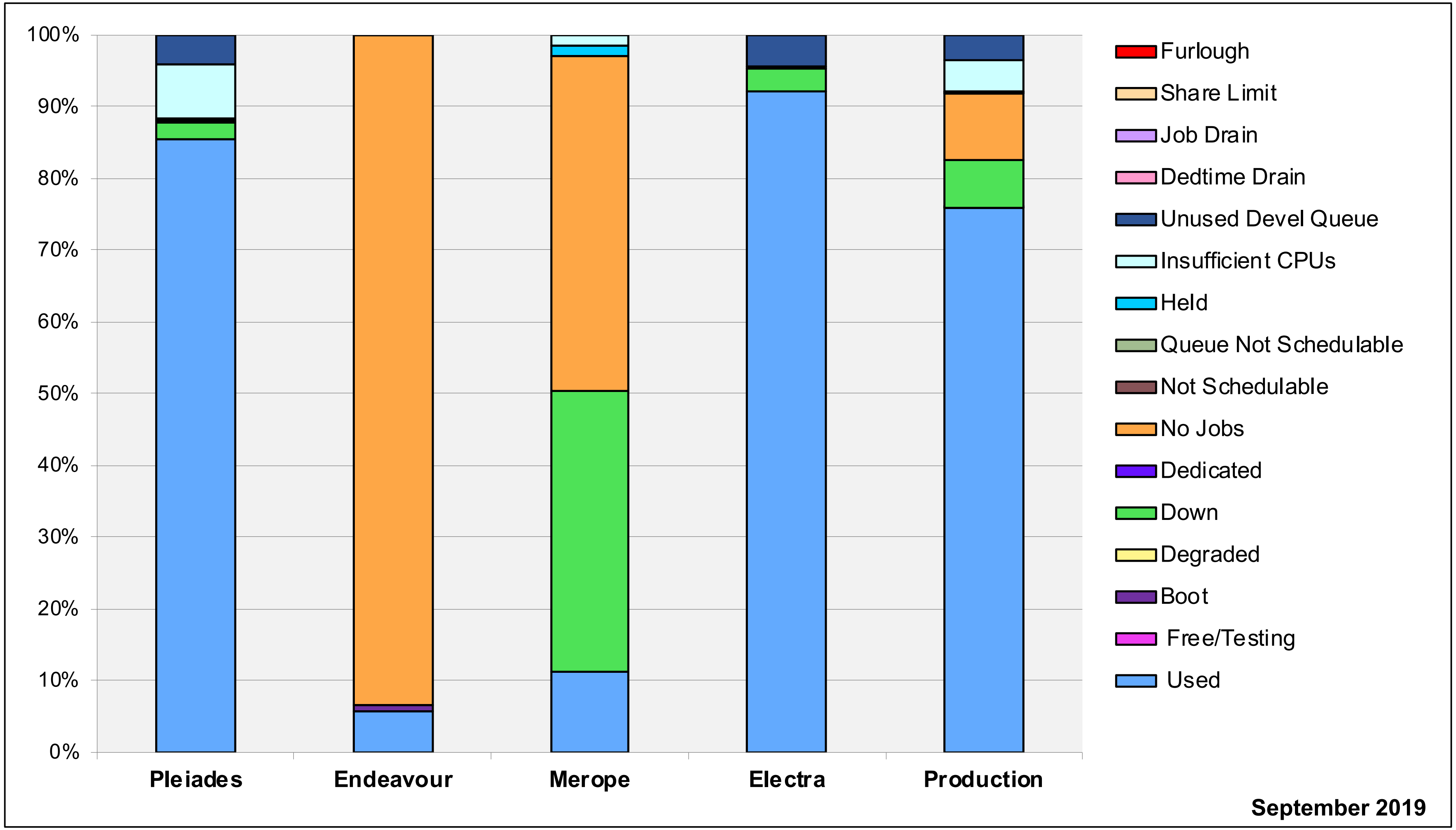
** HECC provided supercomputing resources and services in support of this work*

News and Events

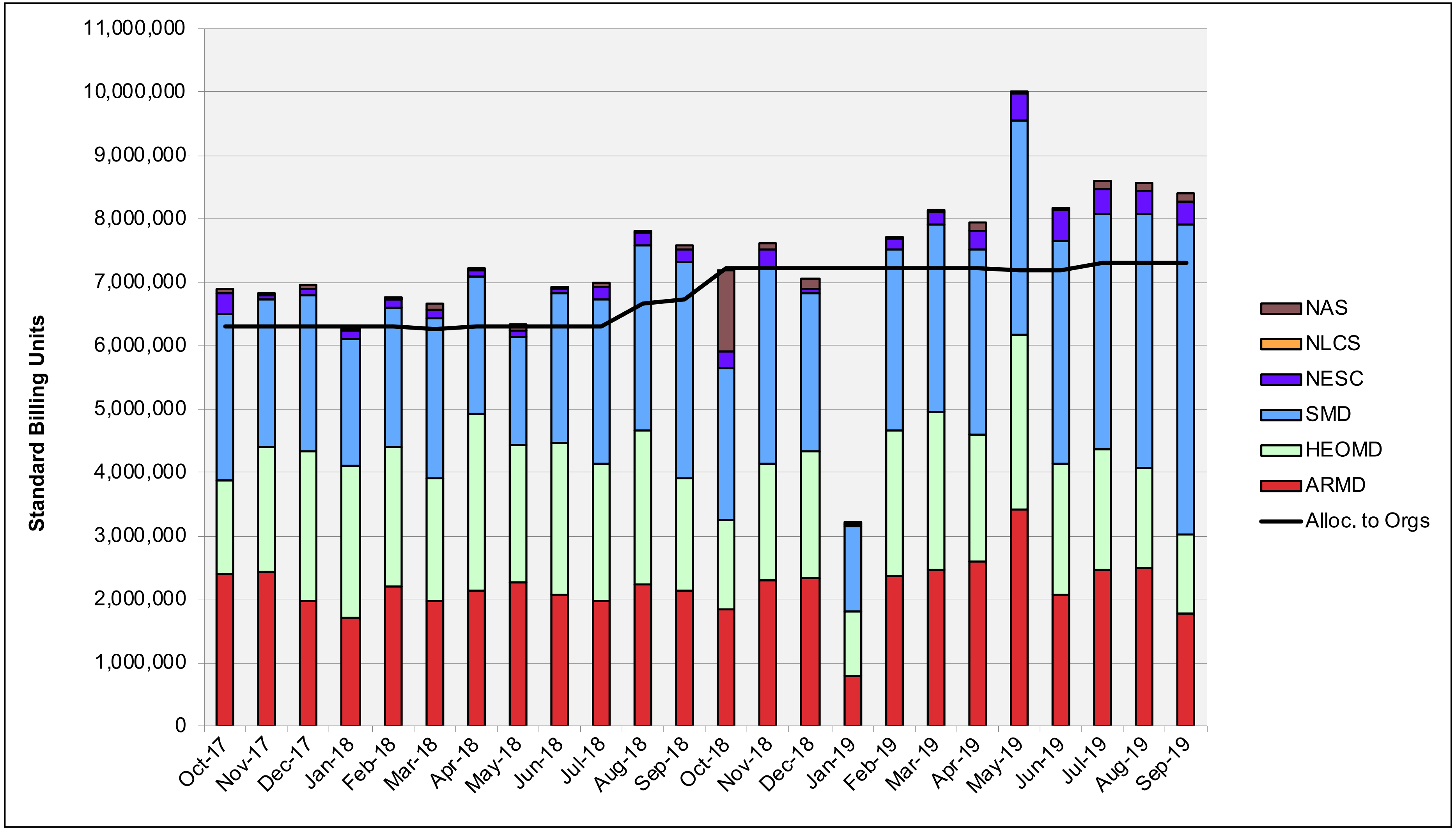
- **We're going to the moon 2024. Here's what NASA's Bay Area branch is contributing to the mission**, *SFGate*, September 5, 2019—SFGate visited NASA's Ames Research Center in Silicon Valley, including the NASA Advanced Supercomputing Facility and its Pleiades supercomputer and unique hyperwall visualization system. *https://www.sfgate.com/science/article/NASA-Ames-Ames-Research-Center-moon-2024-14411263.php#photo-18209032*

- **The Reg chats to HPE's HPC man about NASA's supercomputers, lunar ambitions and Columbia**, *The Register*, September 11, 2019—The Register had a chat with supercomputing veteran Bill Mannel, vice president and general manager of HPC and AI and HPE, who talked about NASA's newest supercomputer, Aitken, at NASA's Ames Research Center in Silicon Valley. https://www.theregister.co.uk/2019/09/11/hpe_aitken/

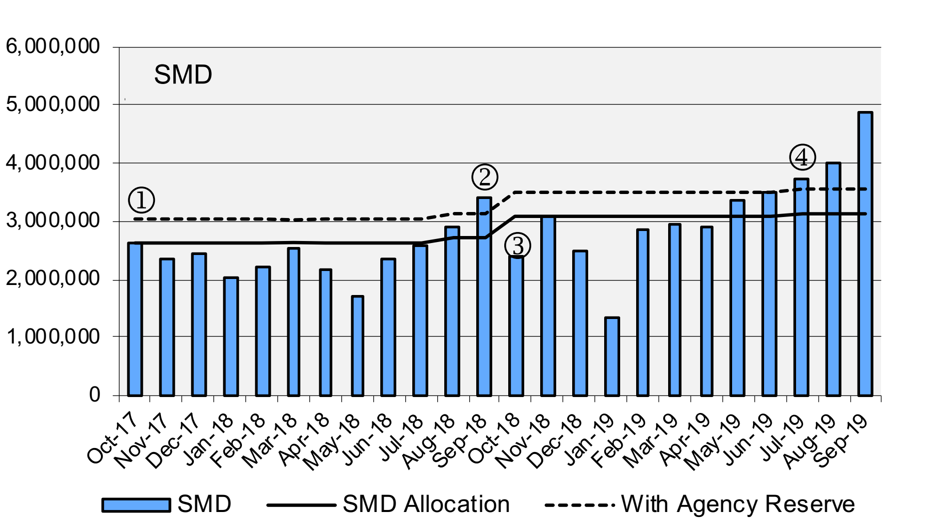
HECC Utilization

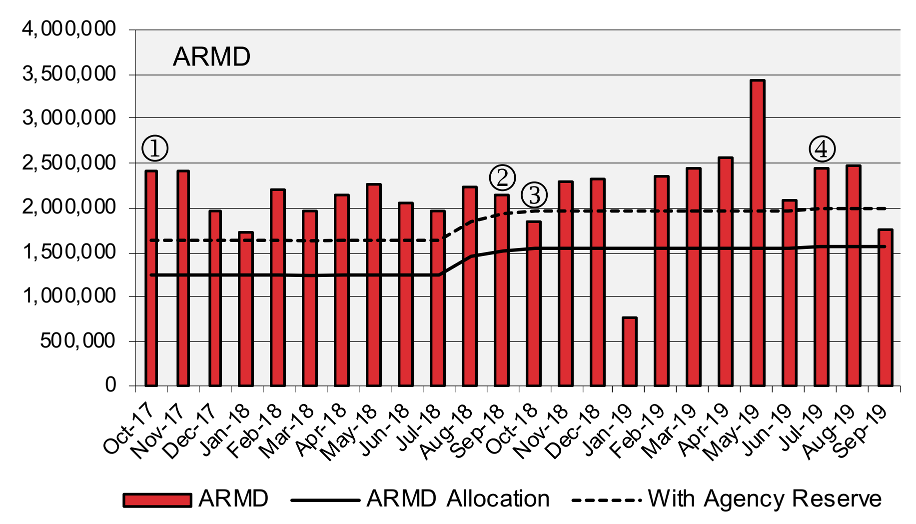


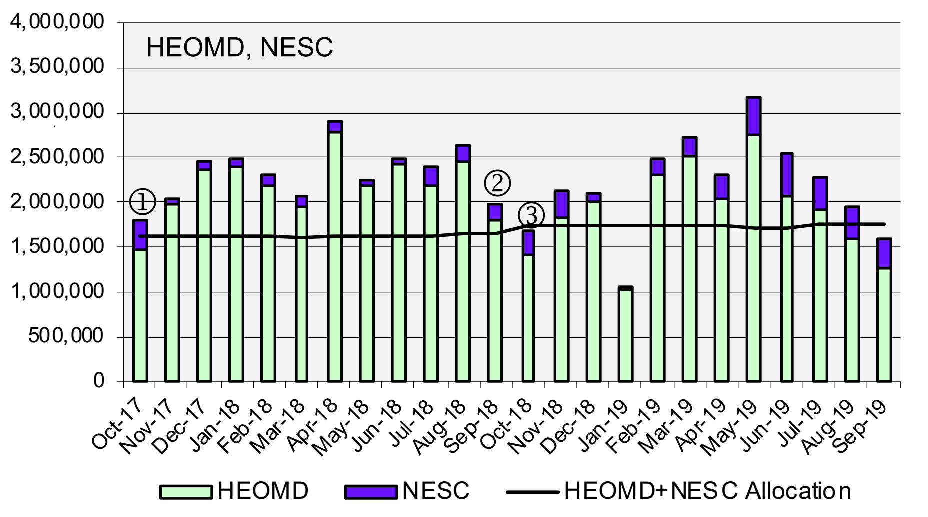
HECC Utilization Normalized to 30-Day Month



HECC Utilization Normalized to 30-Day Month







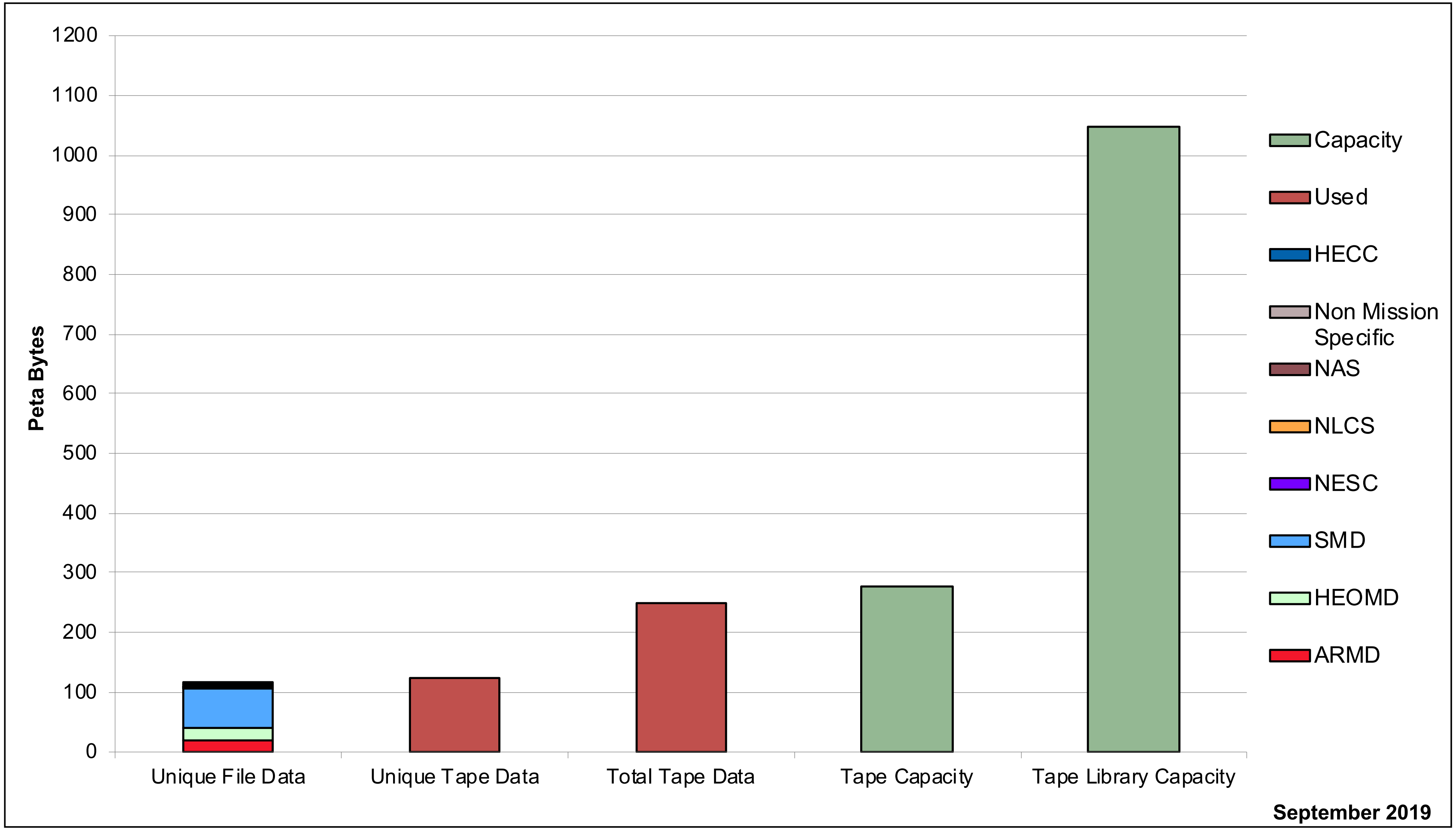
① 4 Skylake E cells (16 D Rack Equivalence) added to Electra

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

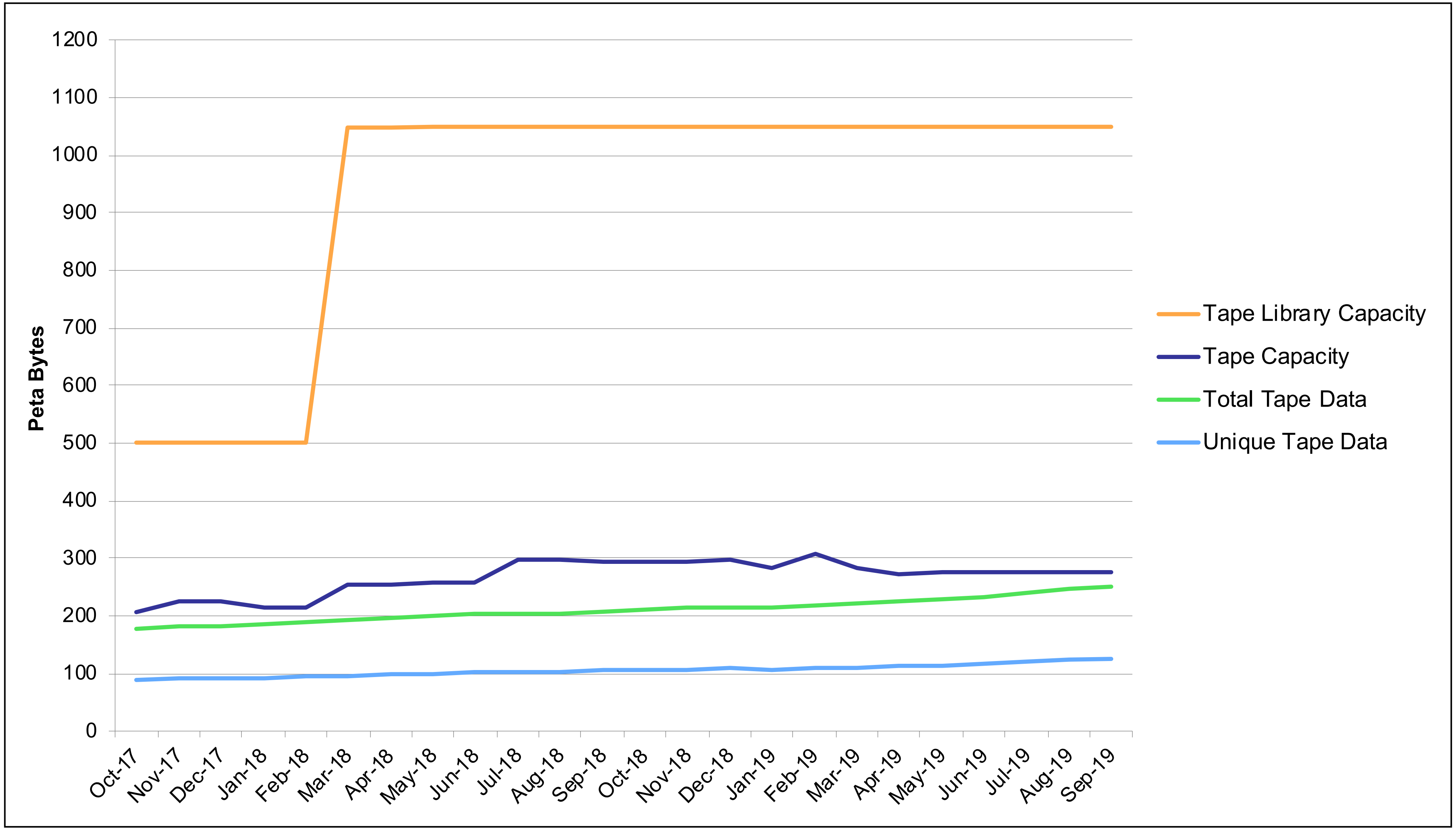
③ 2 Skylake E cells (8 D Rack Equivalence) added to Electra; 1 rack is dedicated to SMD

④ Skylake Tesla GPU V100 Nodes installed

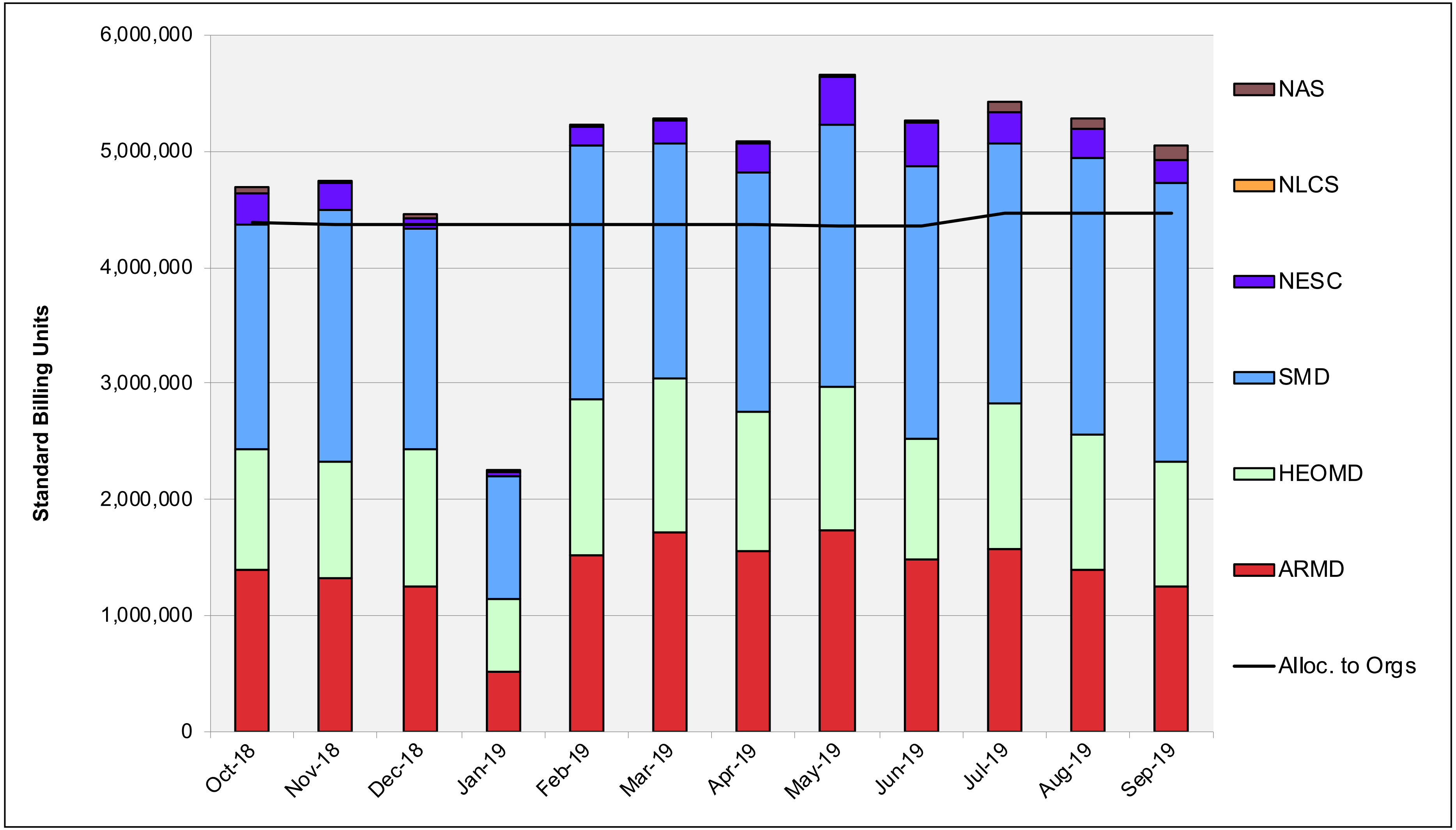
Tape Archive Status



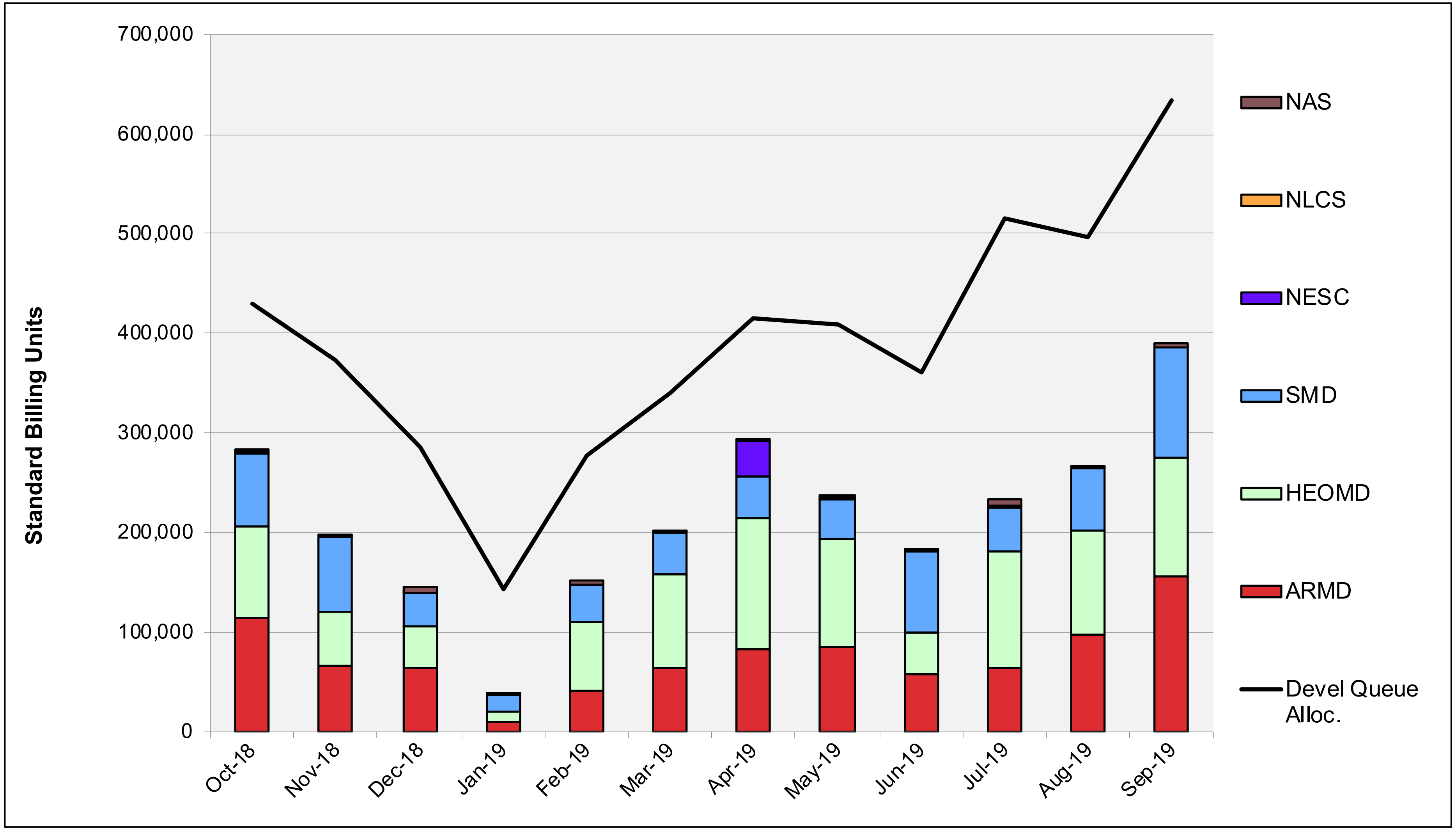
Tape Archive Status



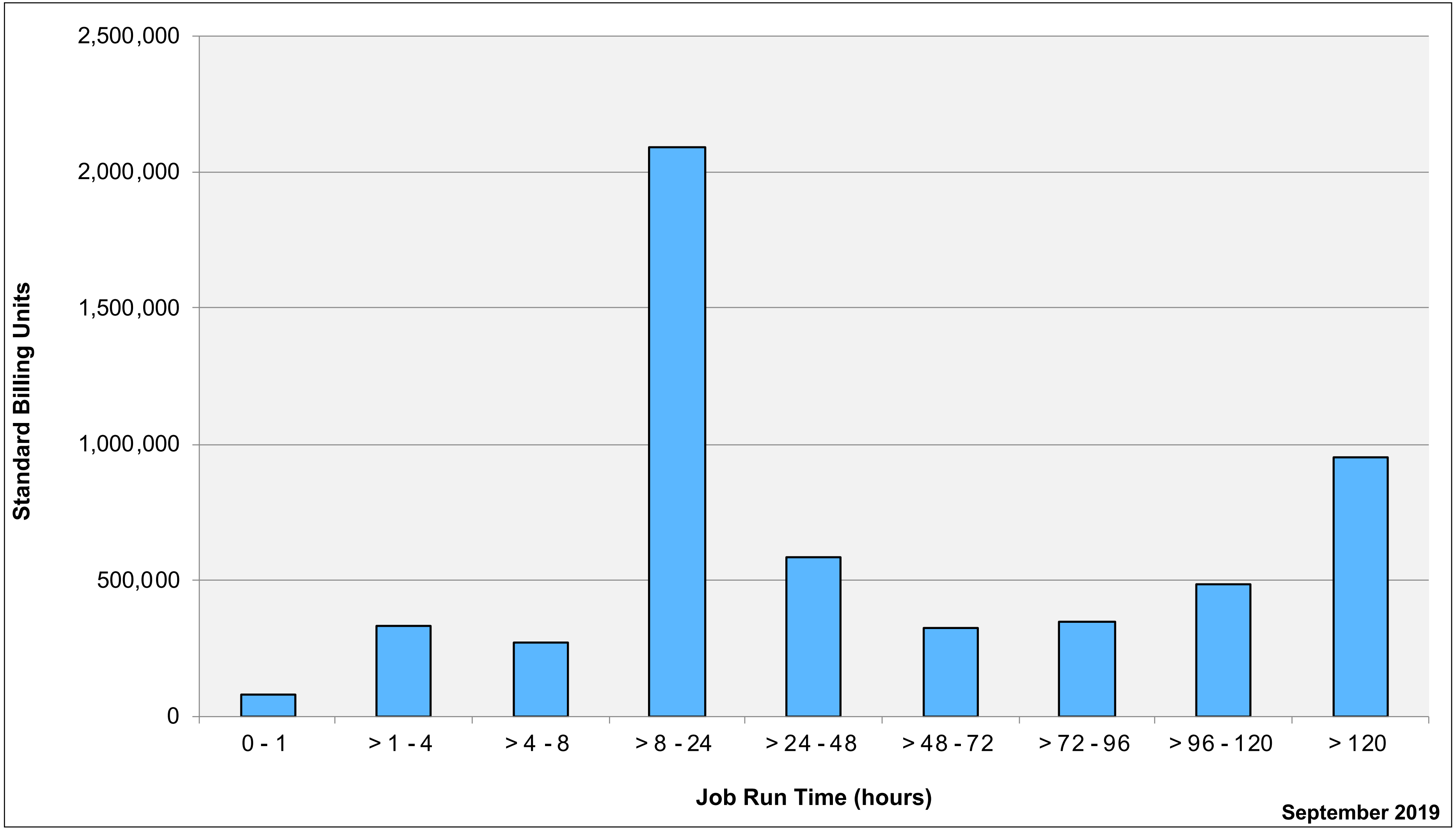
Pleiades: SBUs Reported, Normalized to 30-Day Month



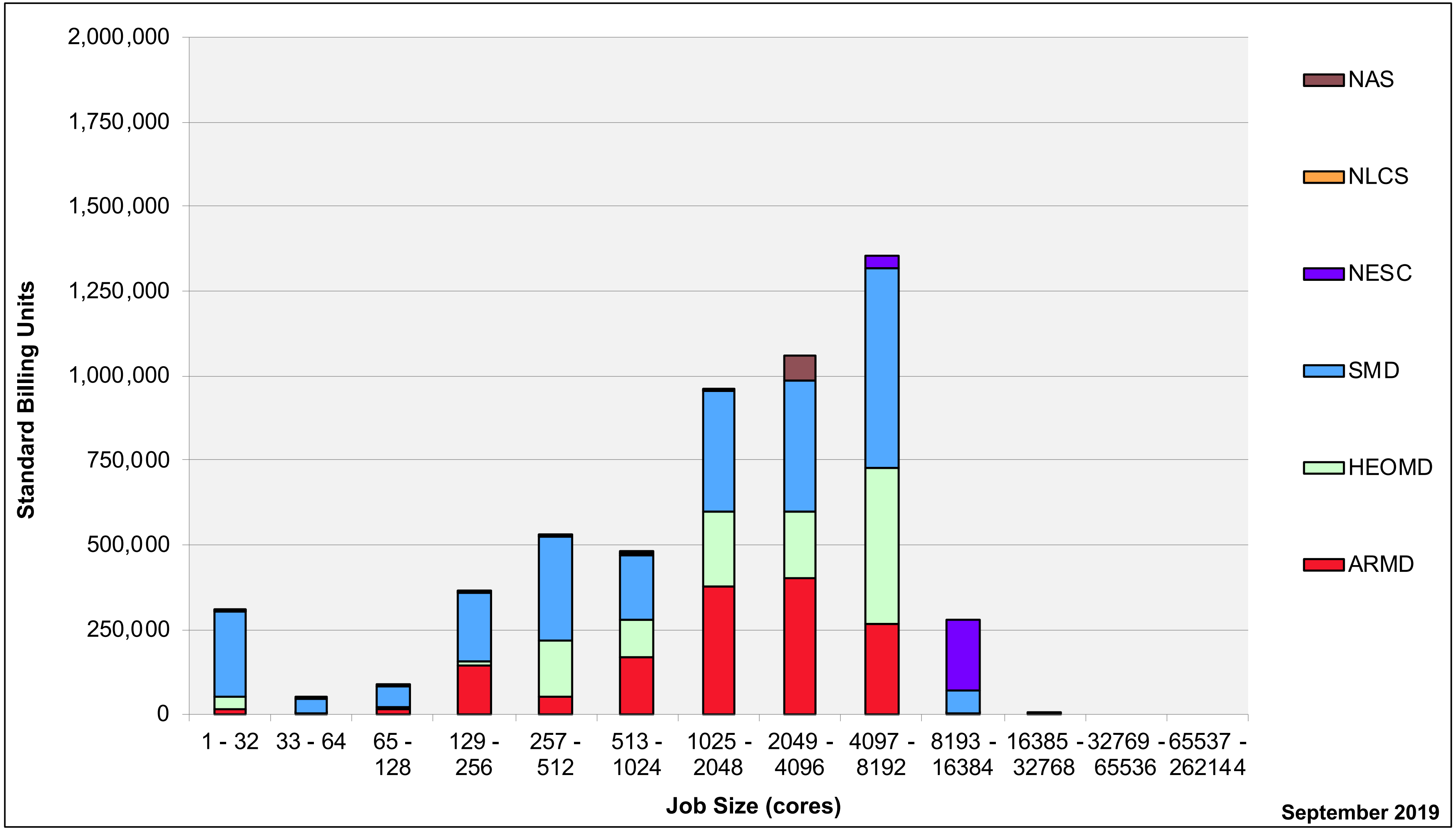
Pleiades: Devel Queue Utilization



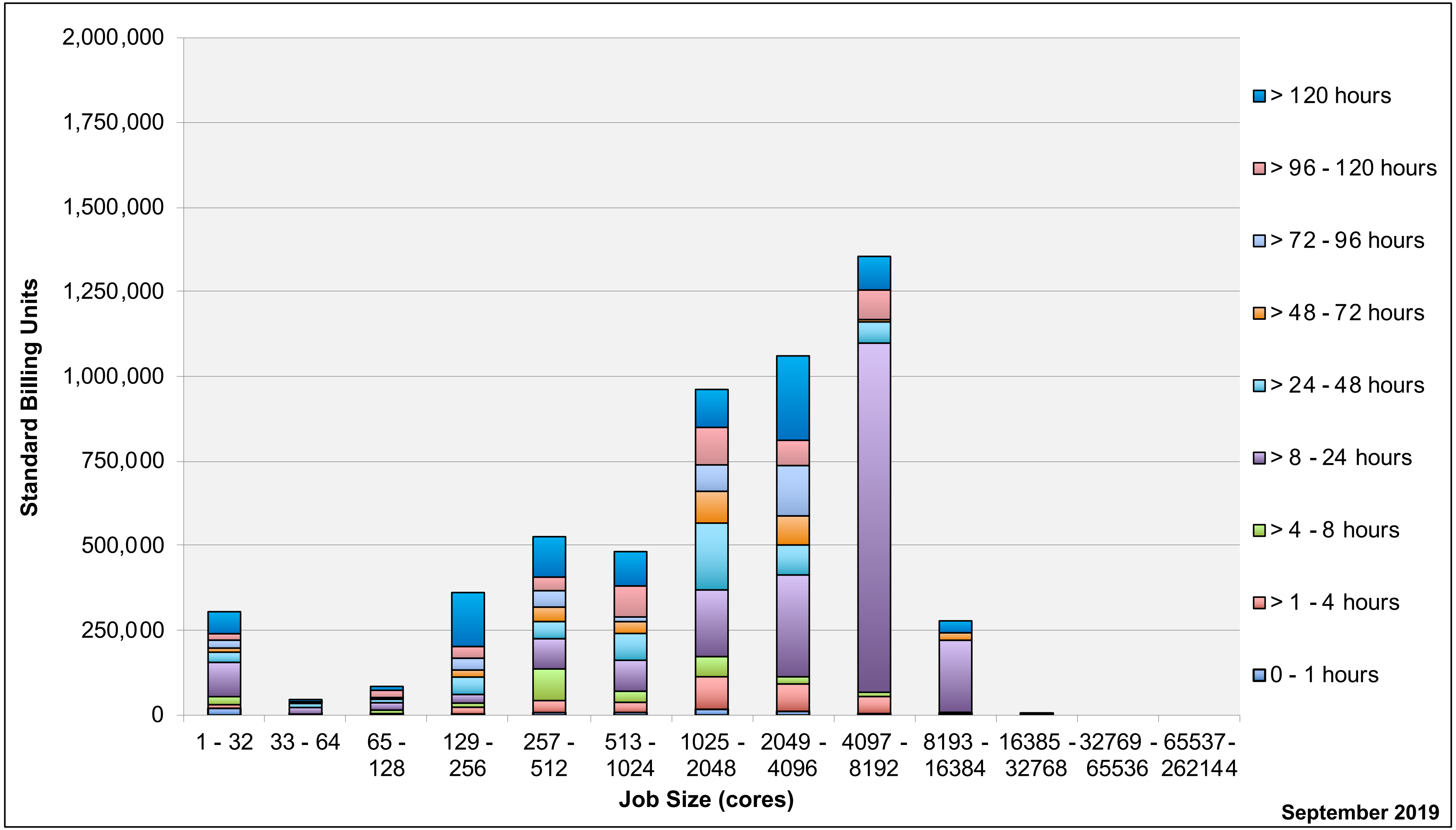
Pleiades: Monthly Utilization by Job Length



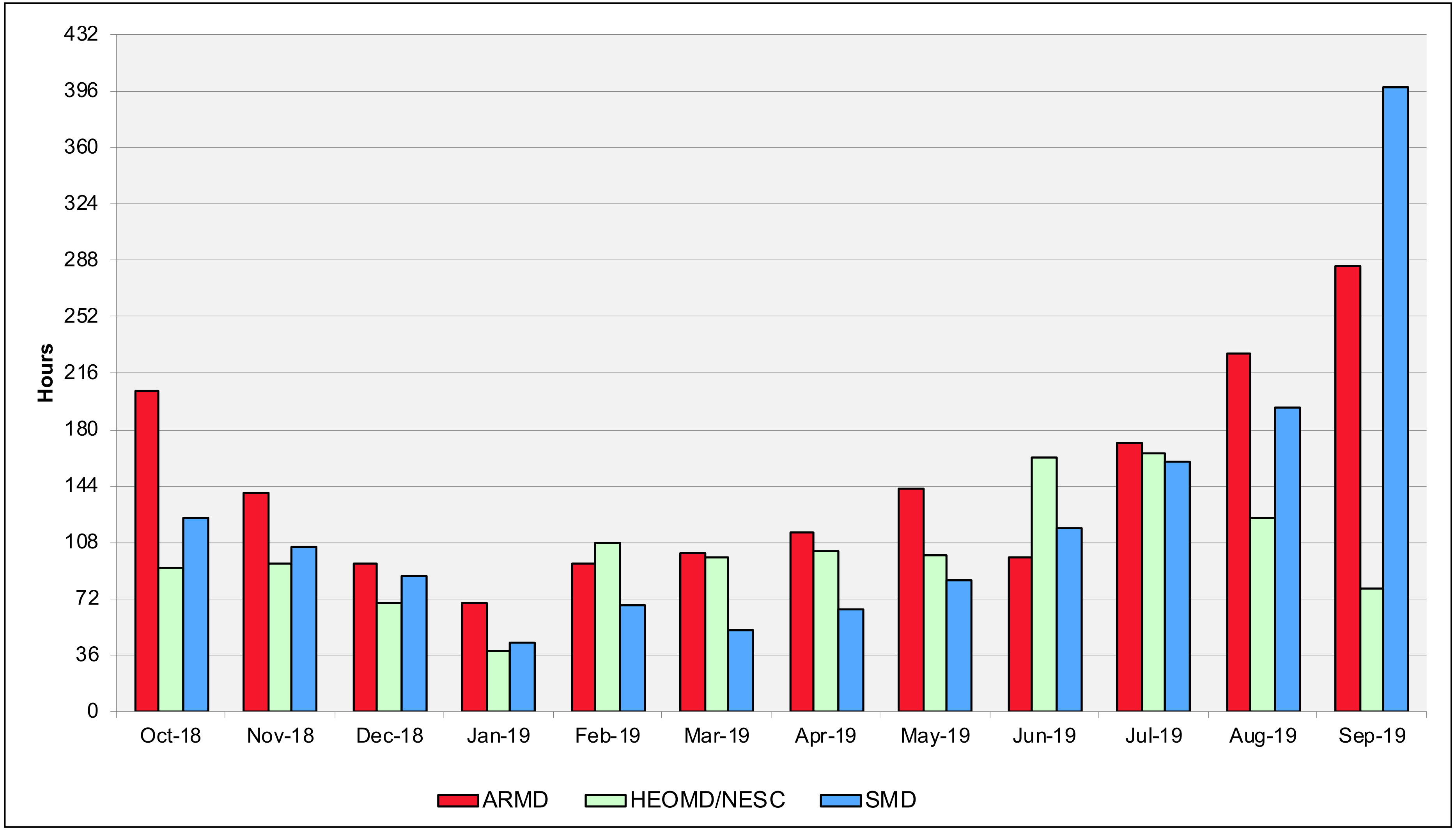
Pleiades: Monthly Utilization by Job Length



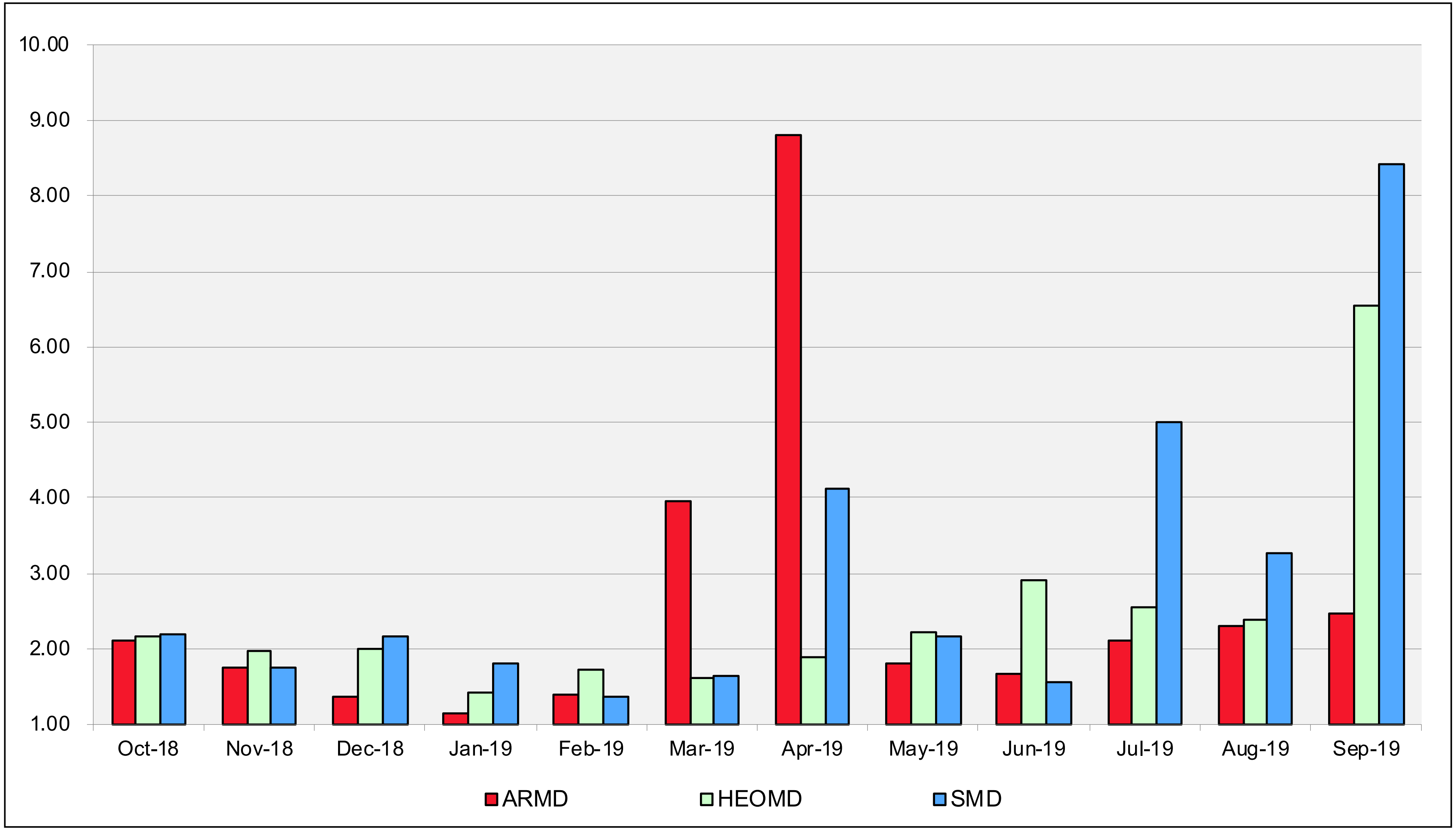
Pleiades: Monthly Utilization by Size and Length



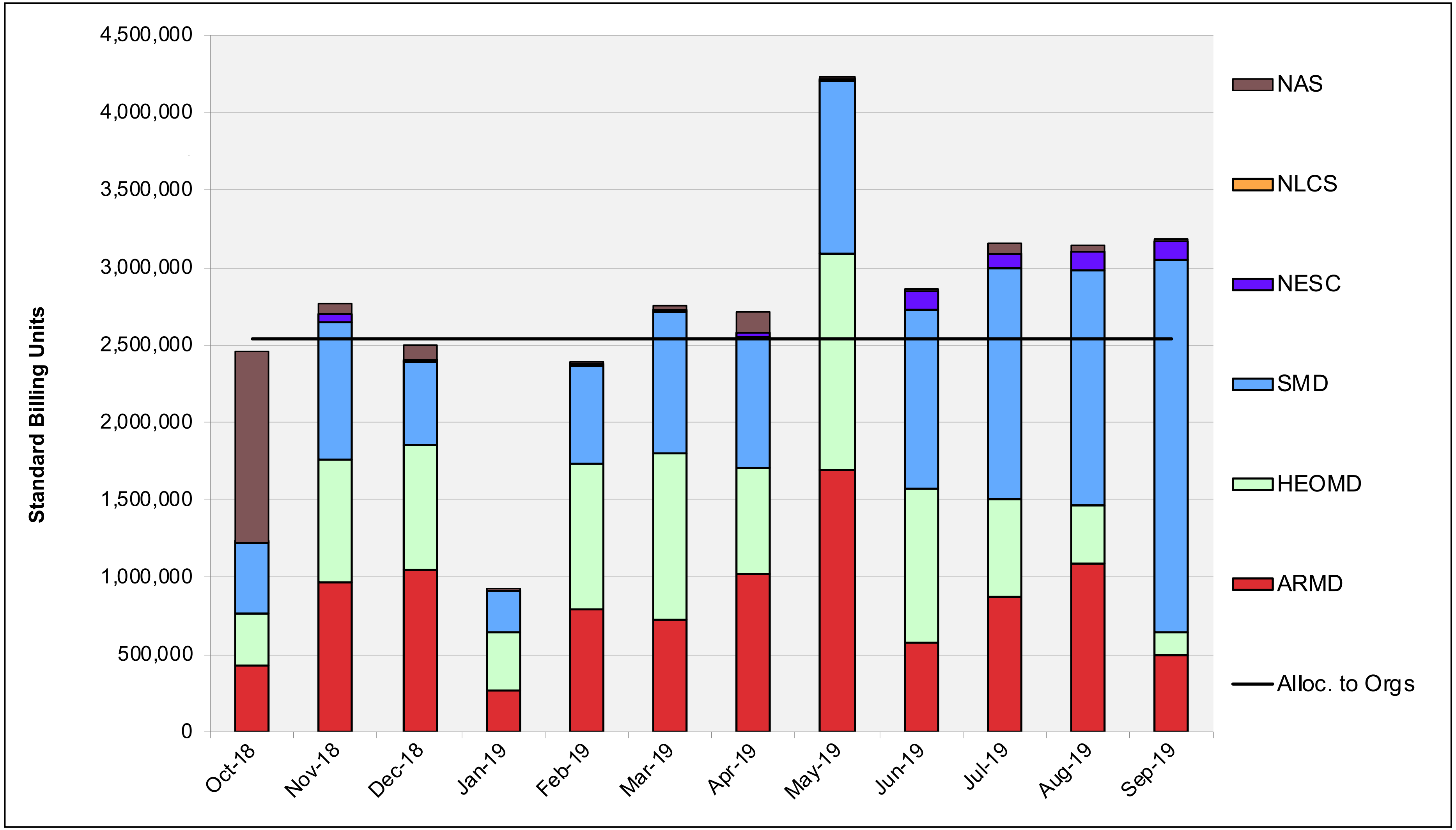
Pleiades: Average Time to Clear All Jobs



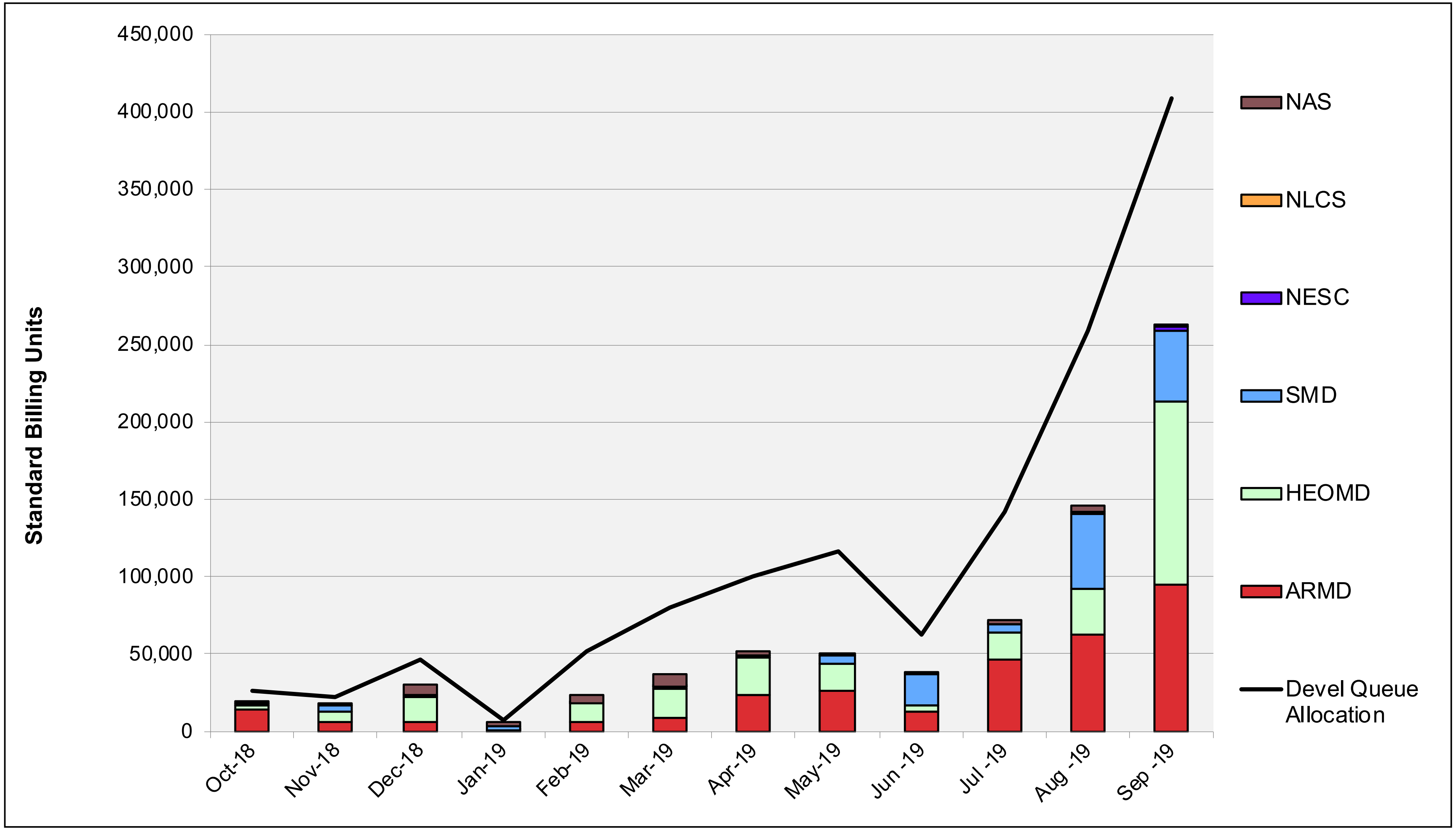
Pleiades: Average Expansion Factor



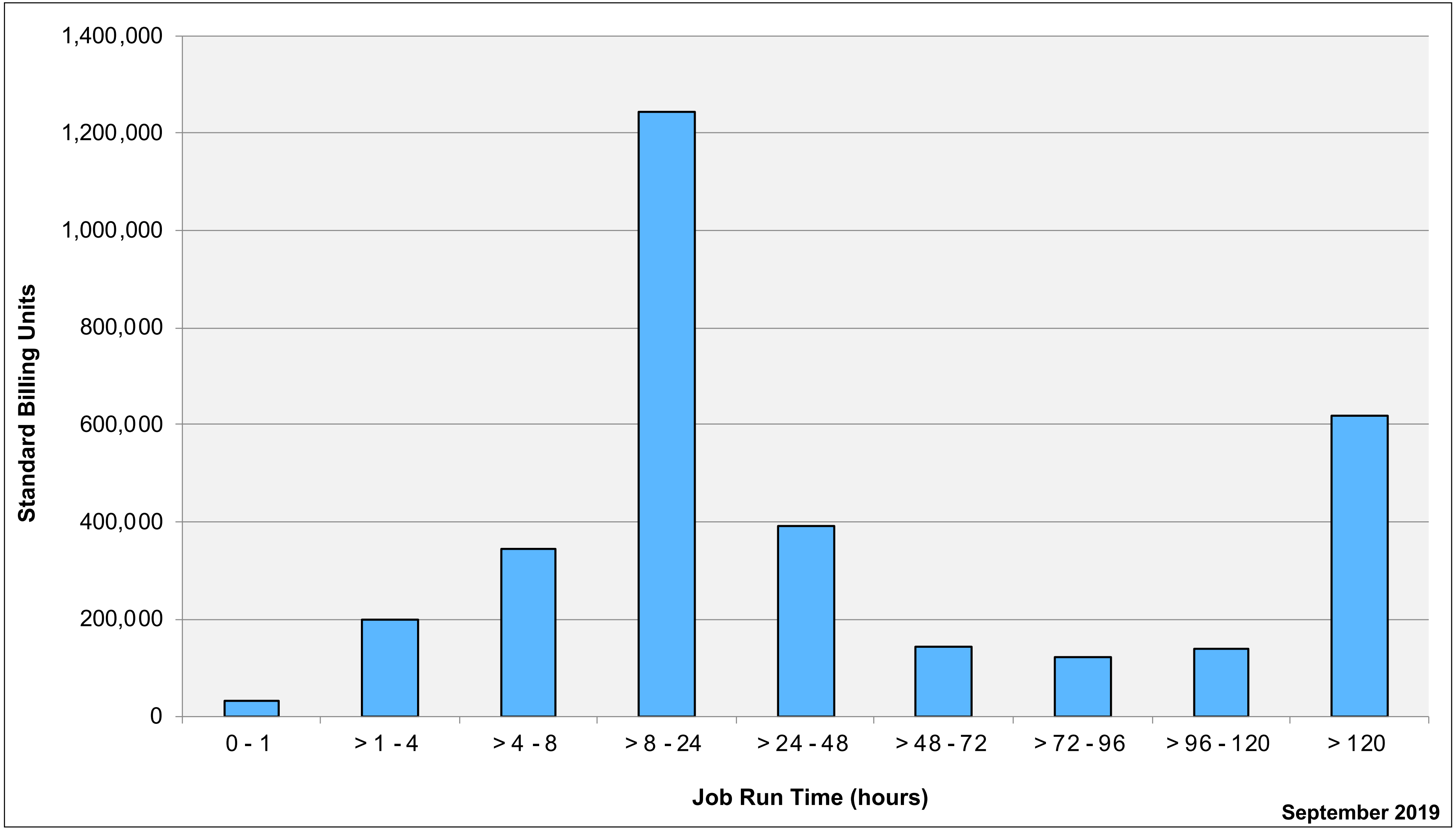
Electra: SBUs Reported, Normalized to 30-Day Month



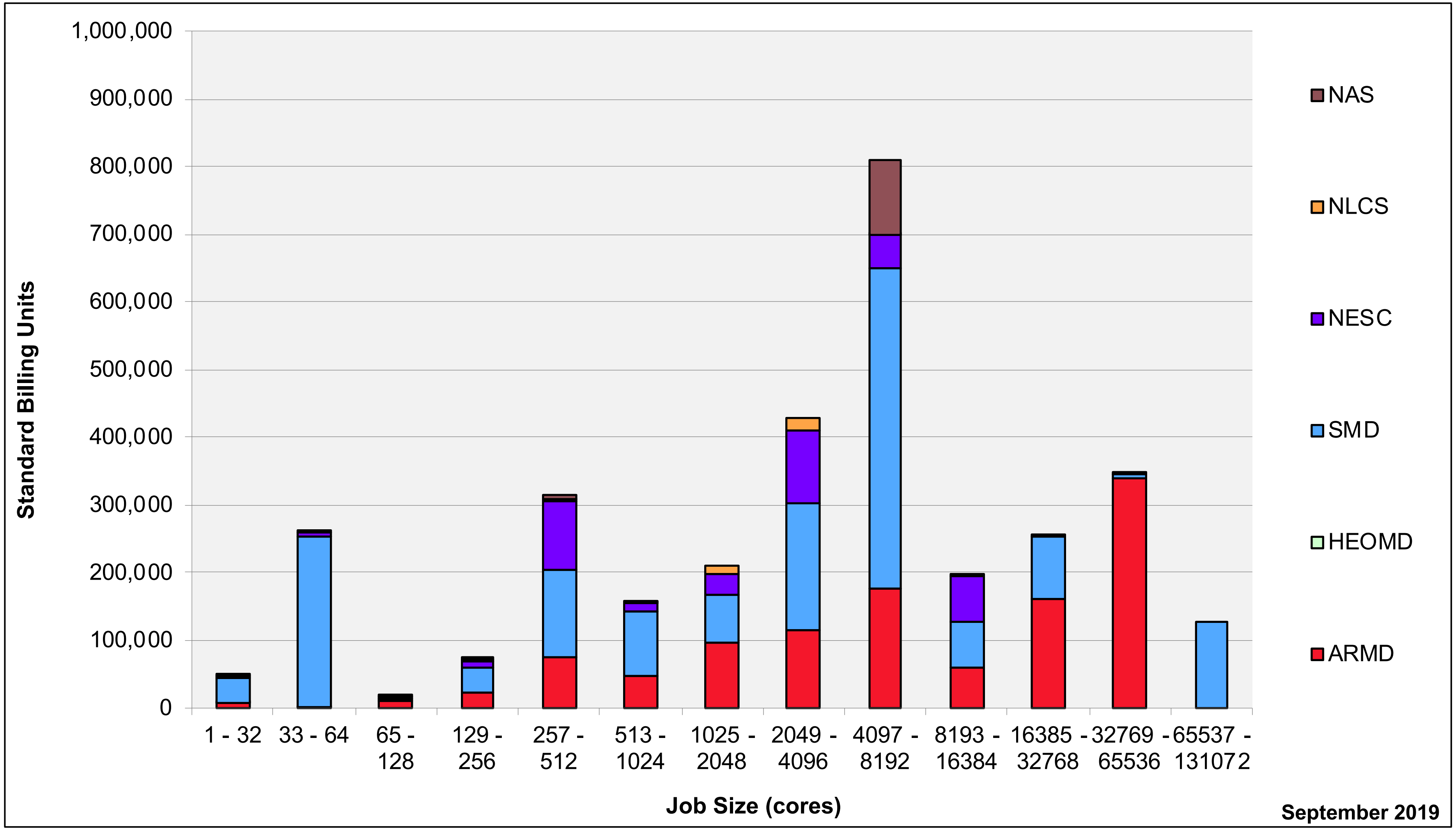
Electra: Devel Queue Utilization



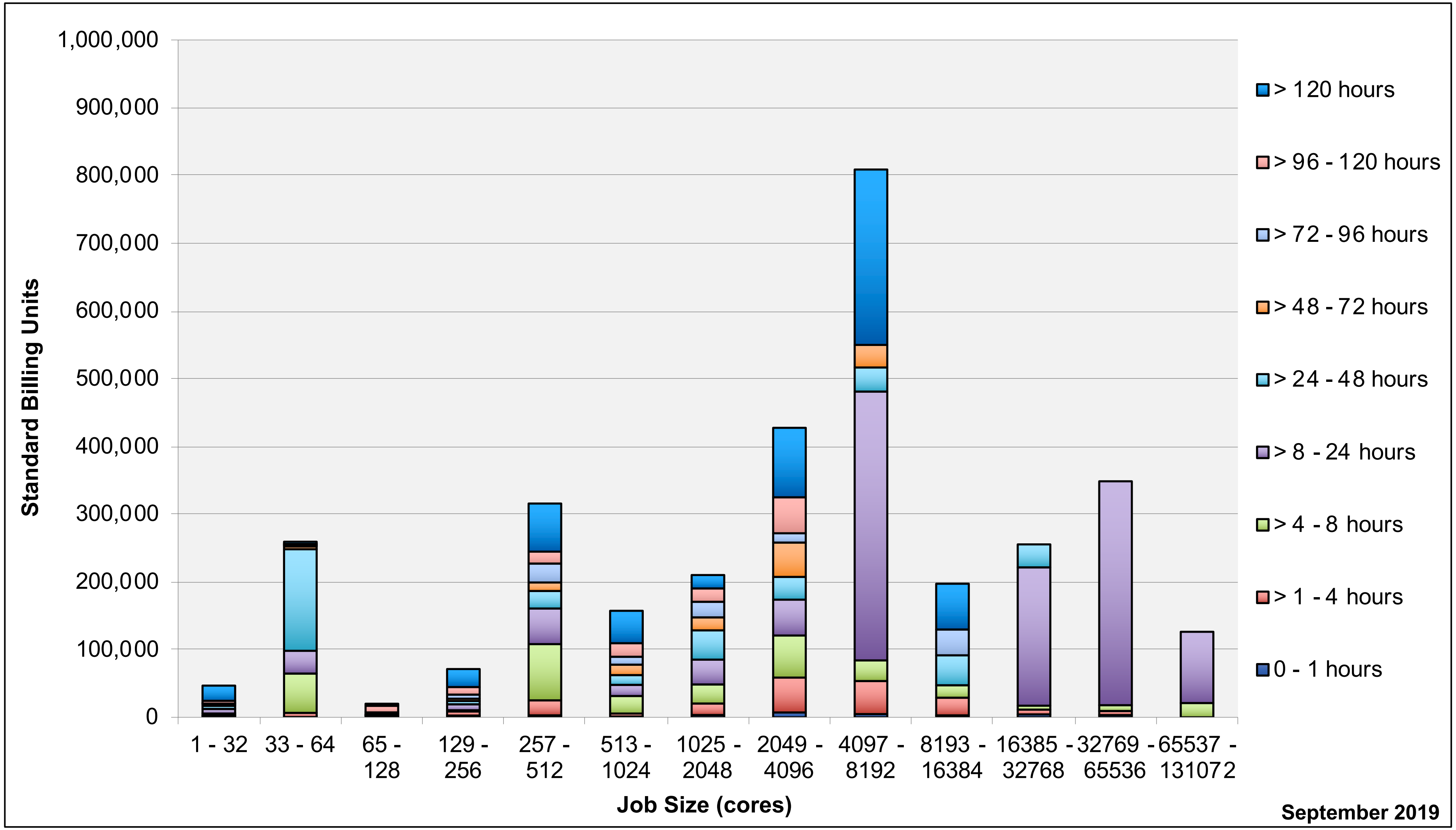
Electra: Monthly Utilization by Job Length



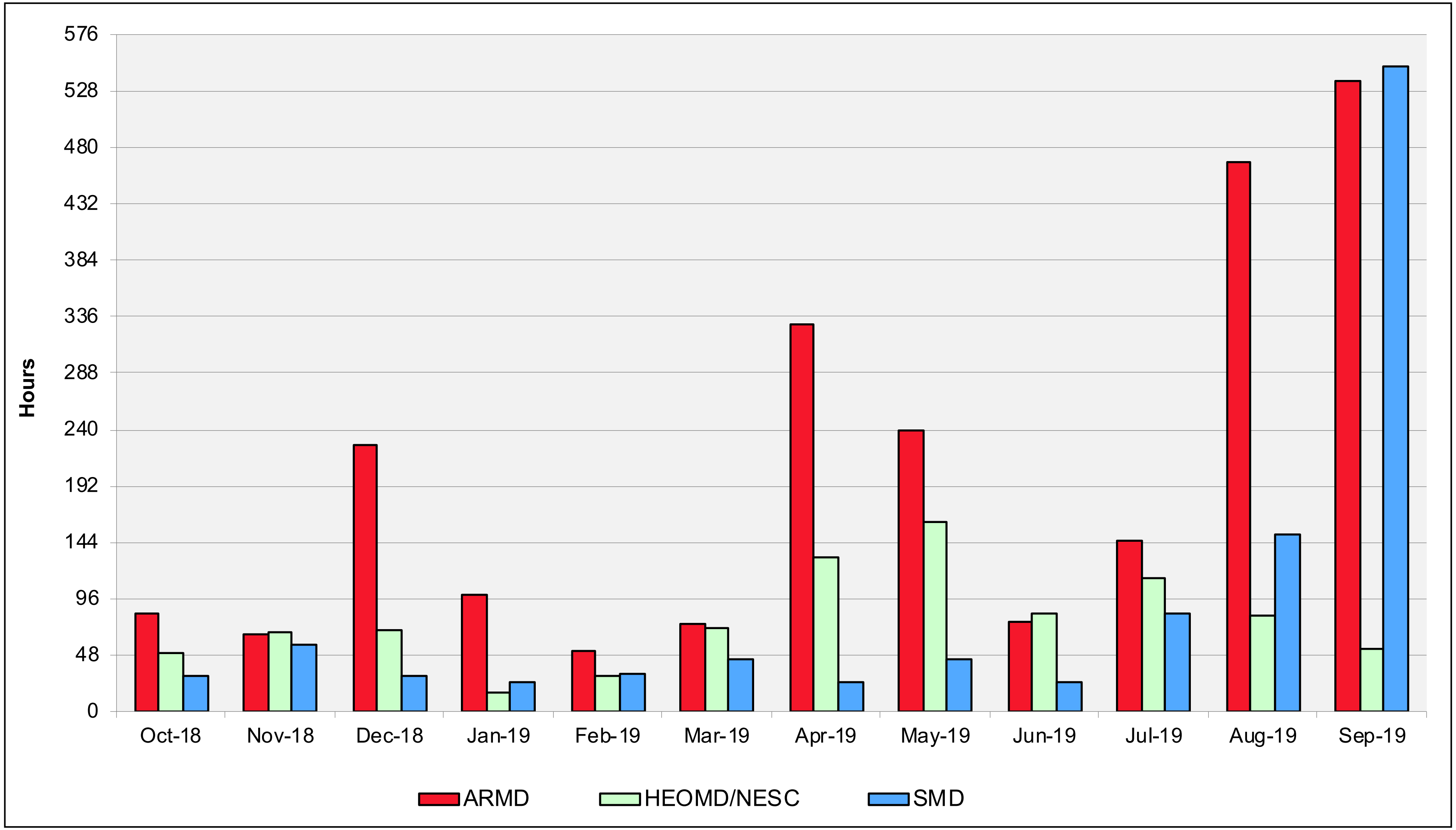
Electra: Monthly Utilization by Job Length



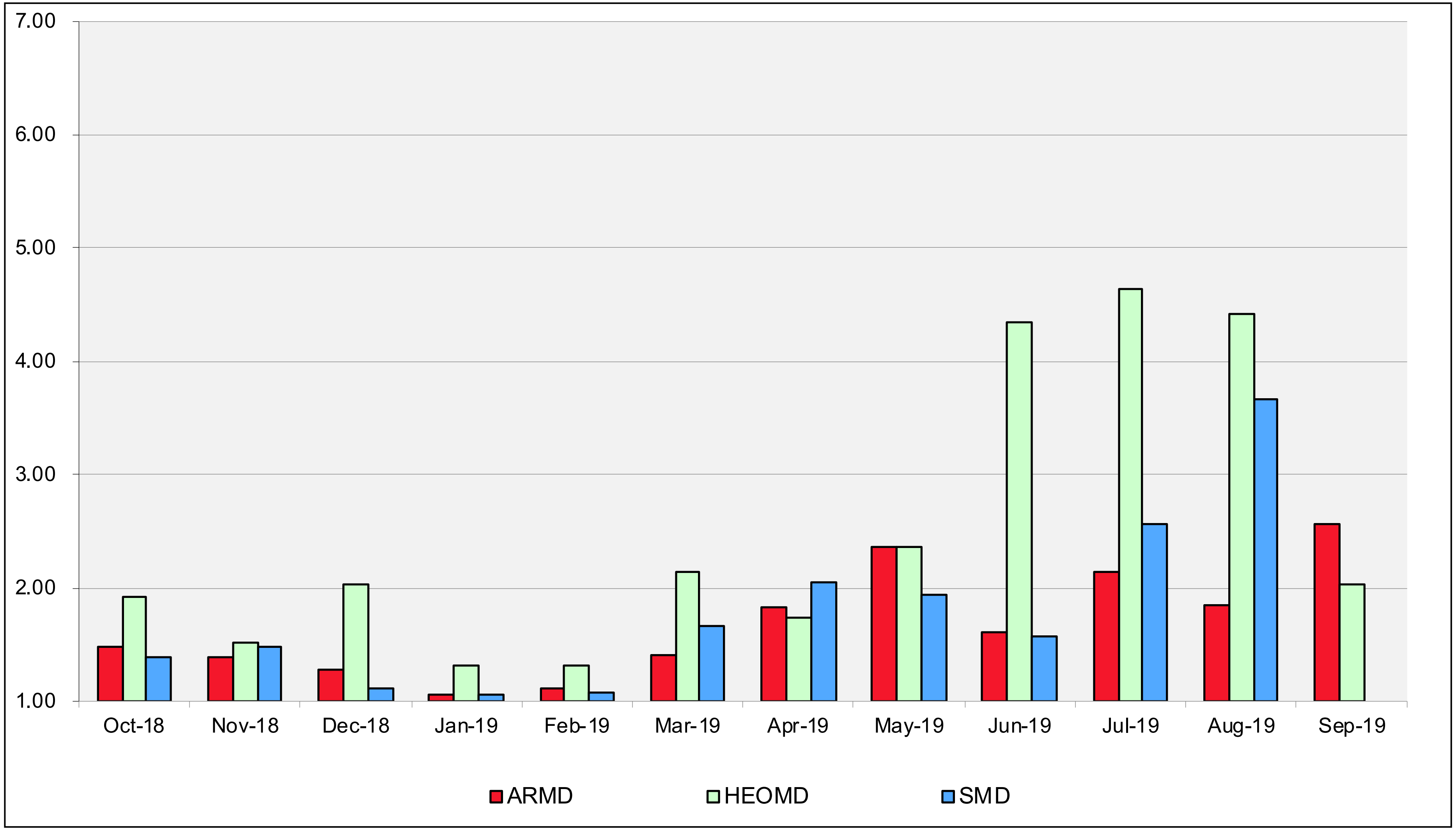
Electra: Monthly Utilization by Size and Length



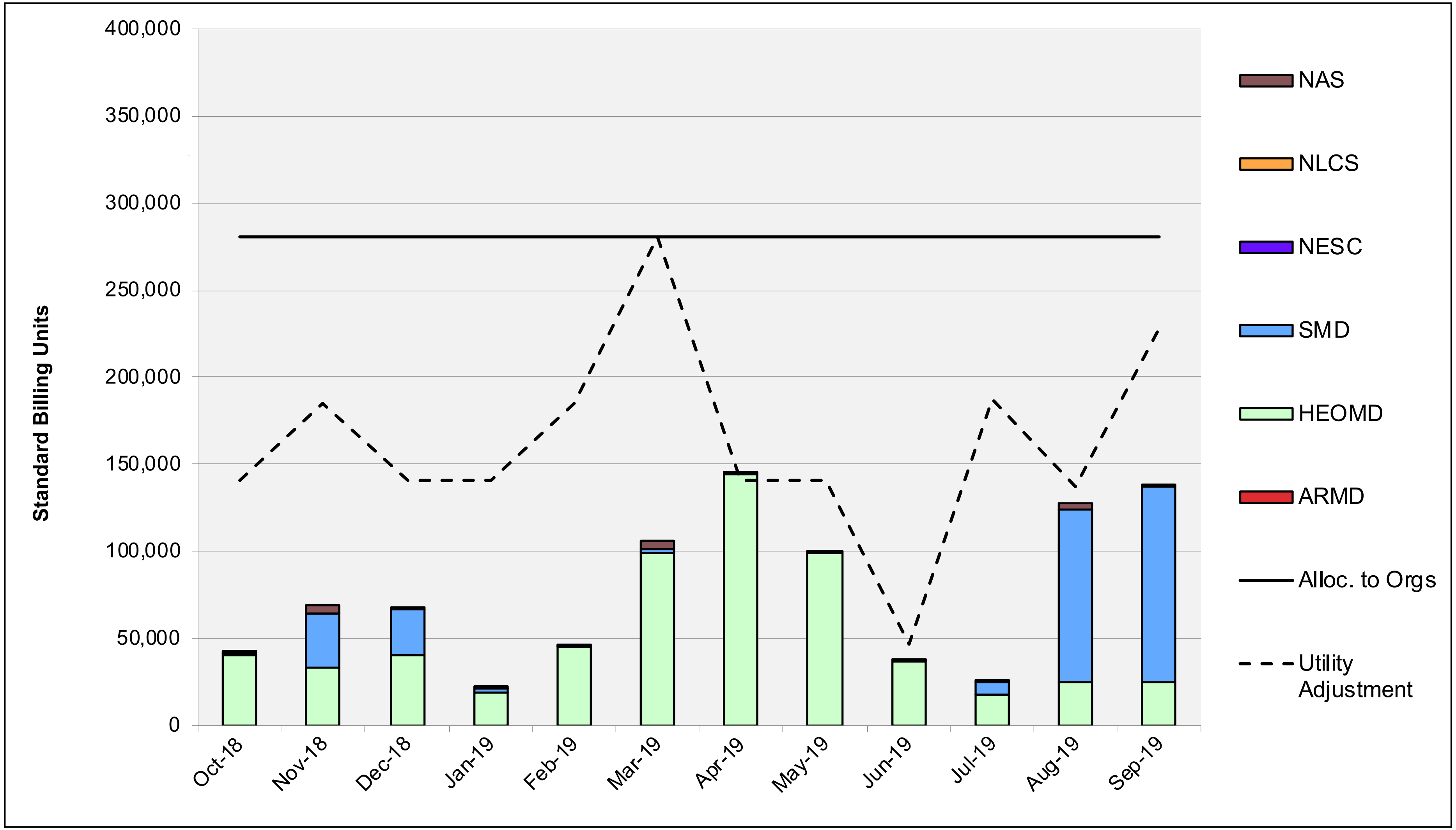
Electra: Average Time to Clear All Jobs



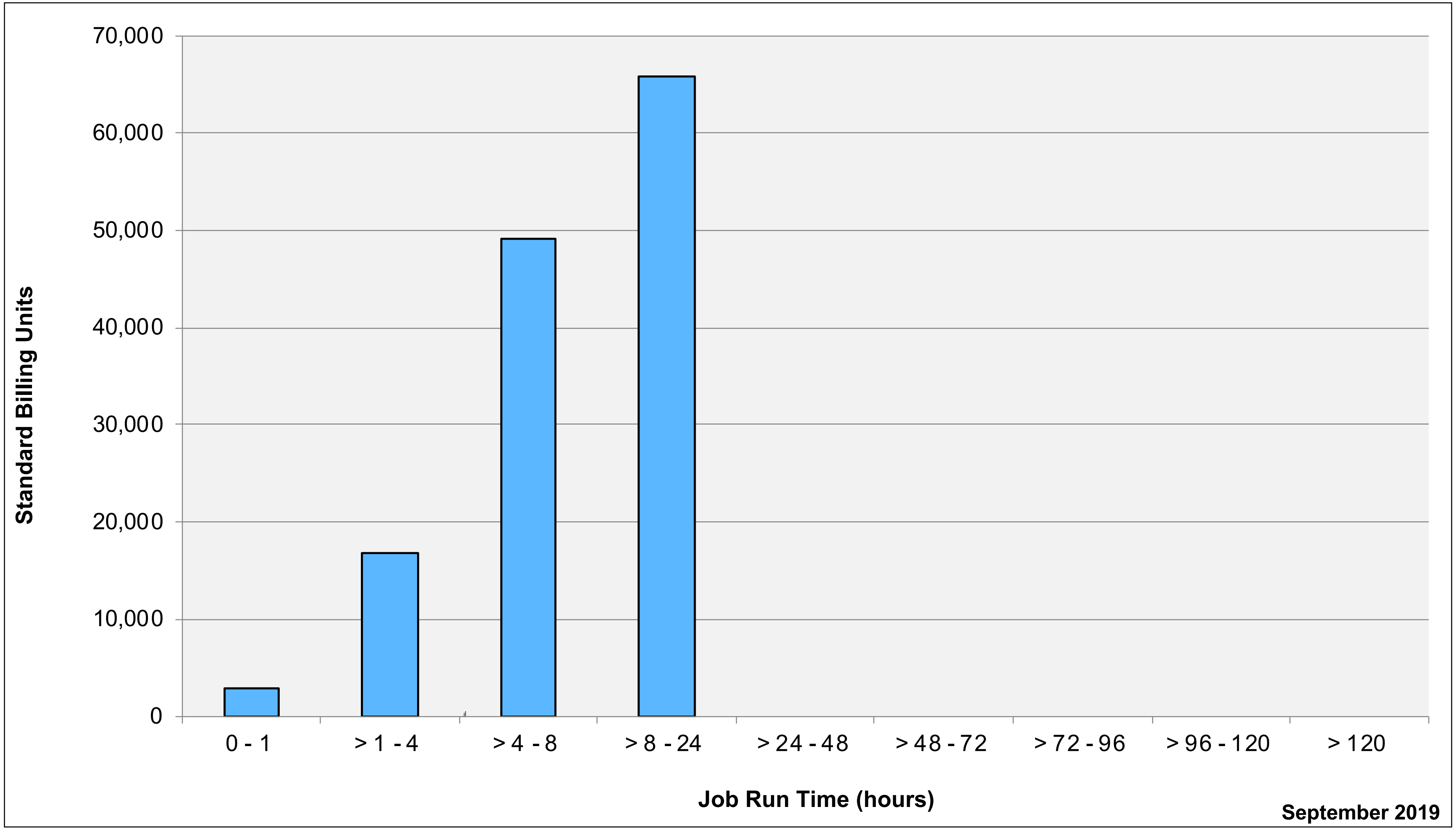
Electra: Average Expansion Factor



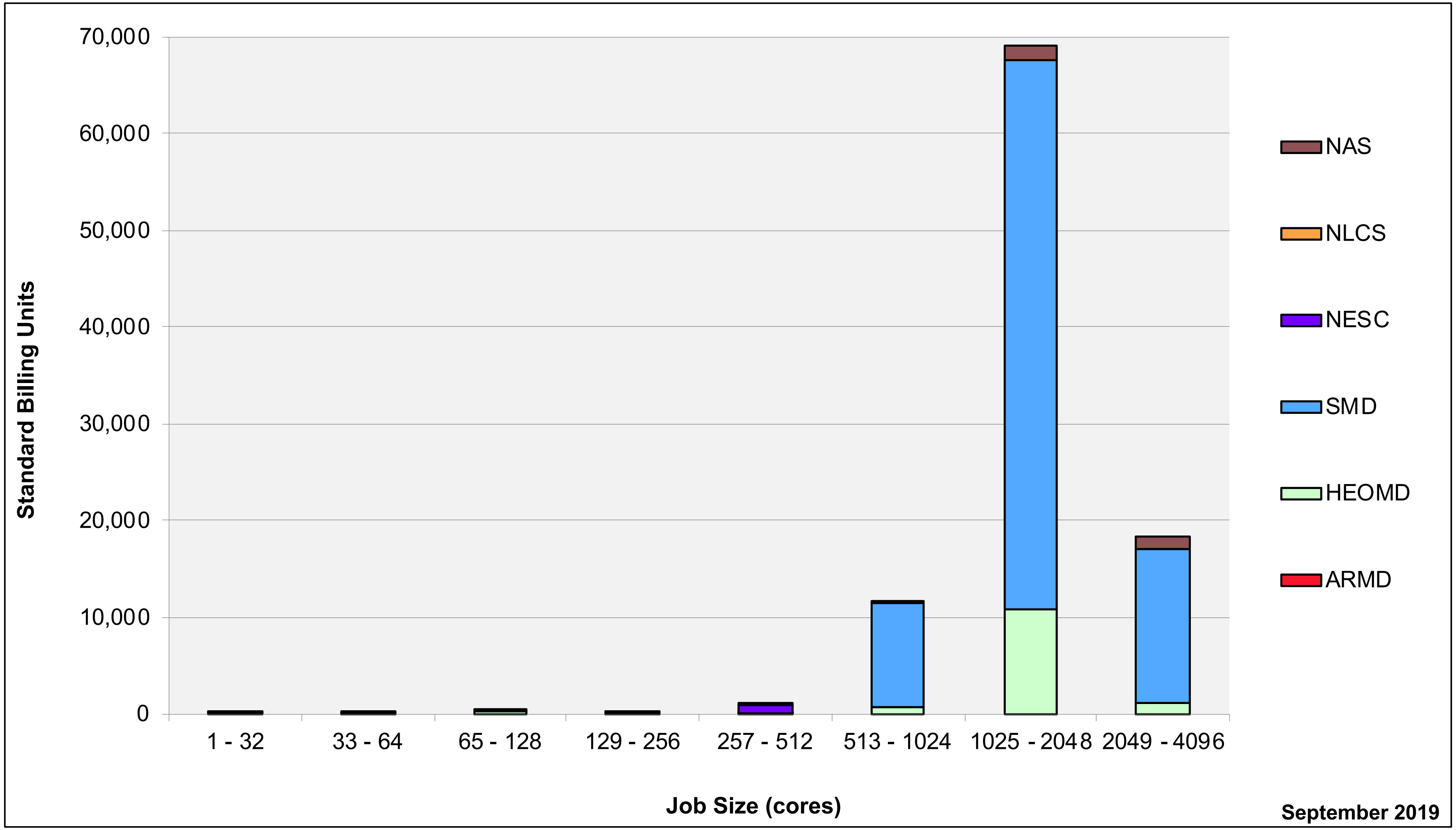
Merope: SBUs Reported, Normalized to 30-Day Month



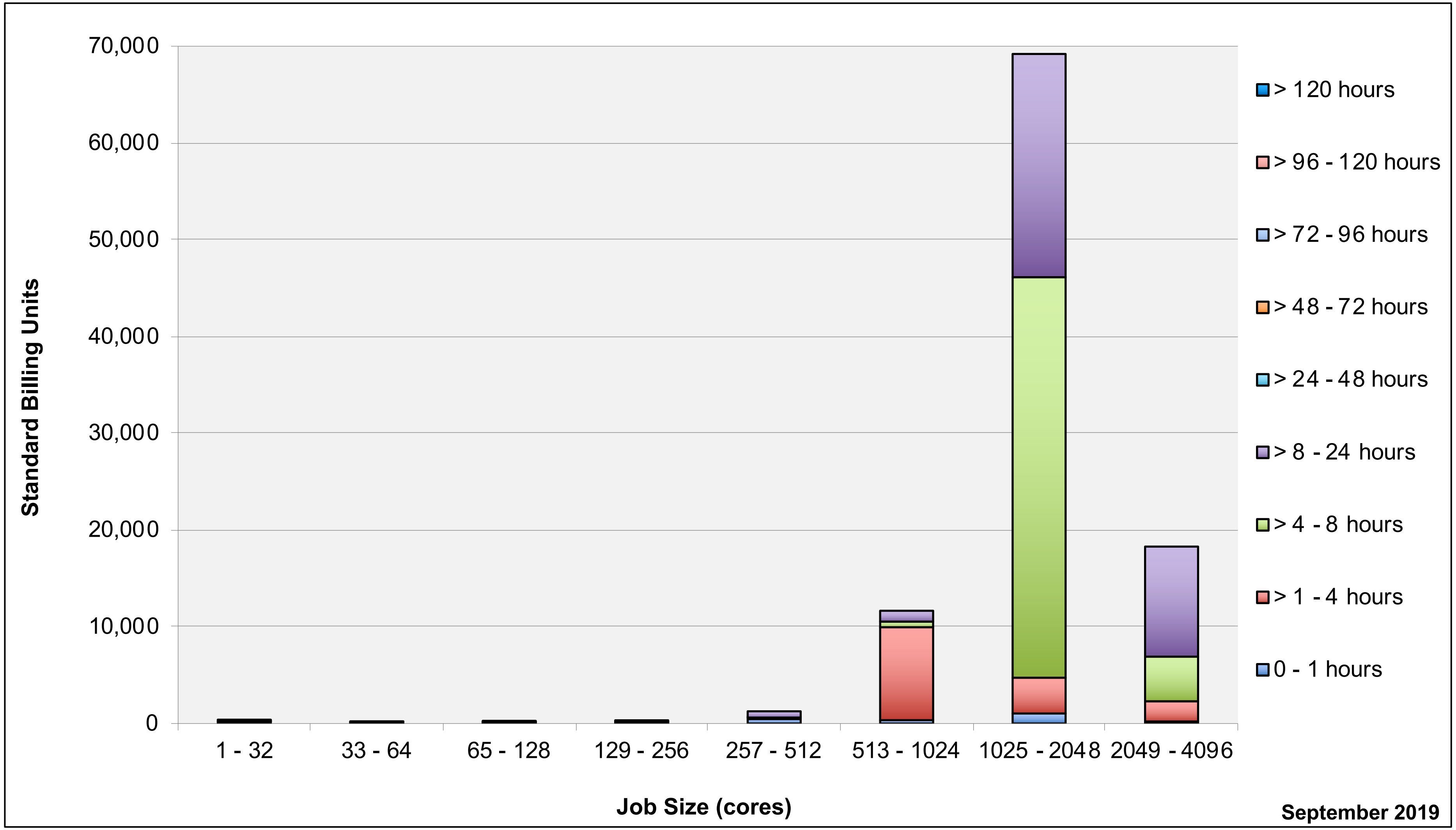
Merope: Monthly Utilization by Job Length



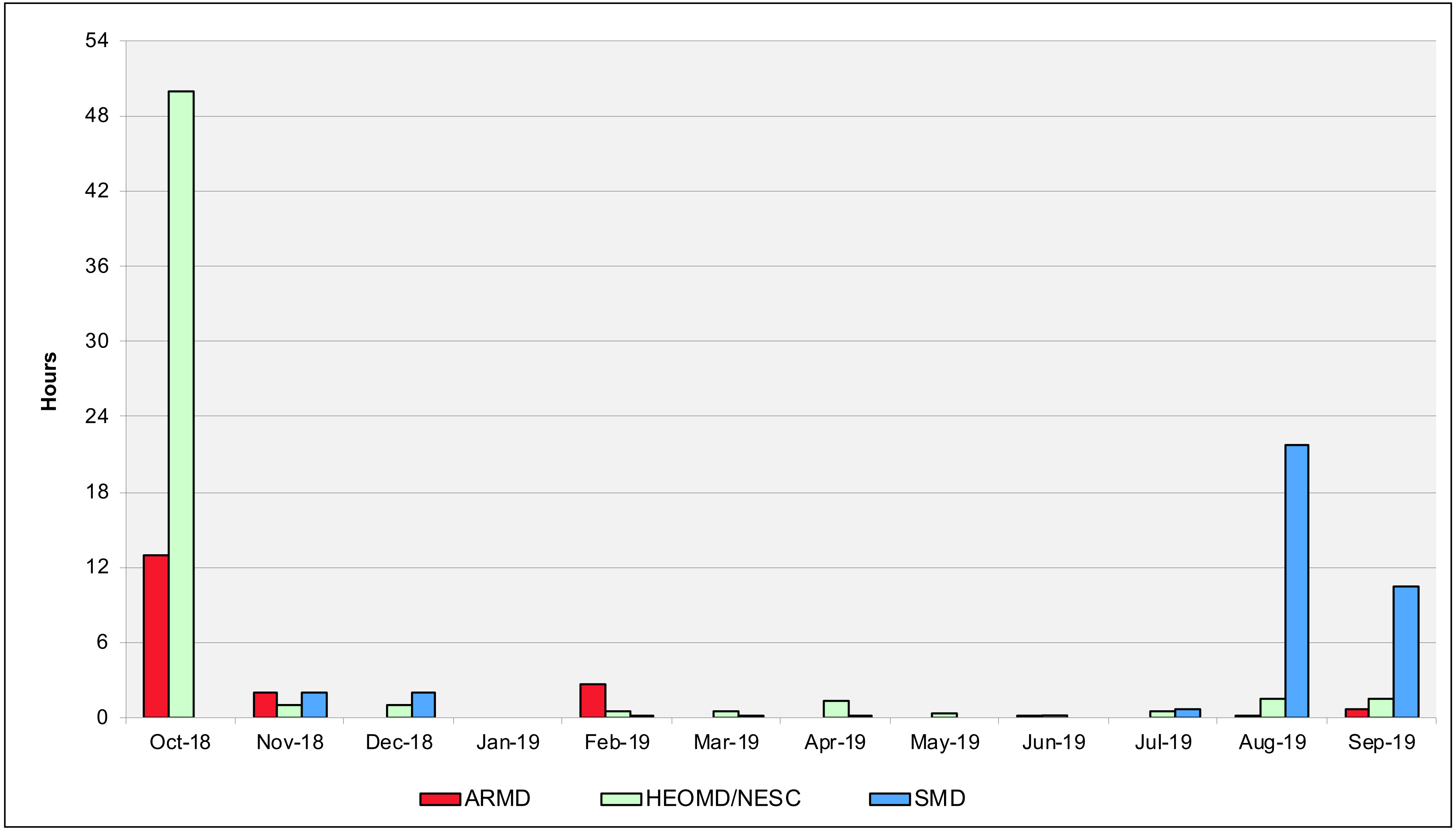
Merope: Monthly Utilization by Job Length



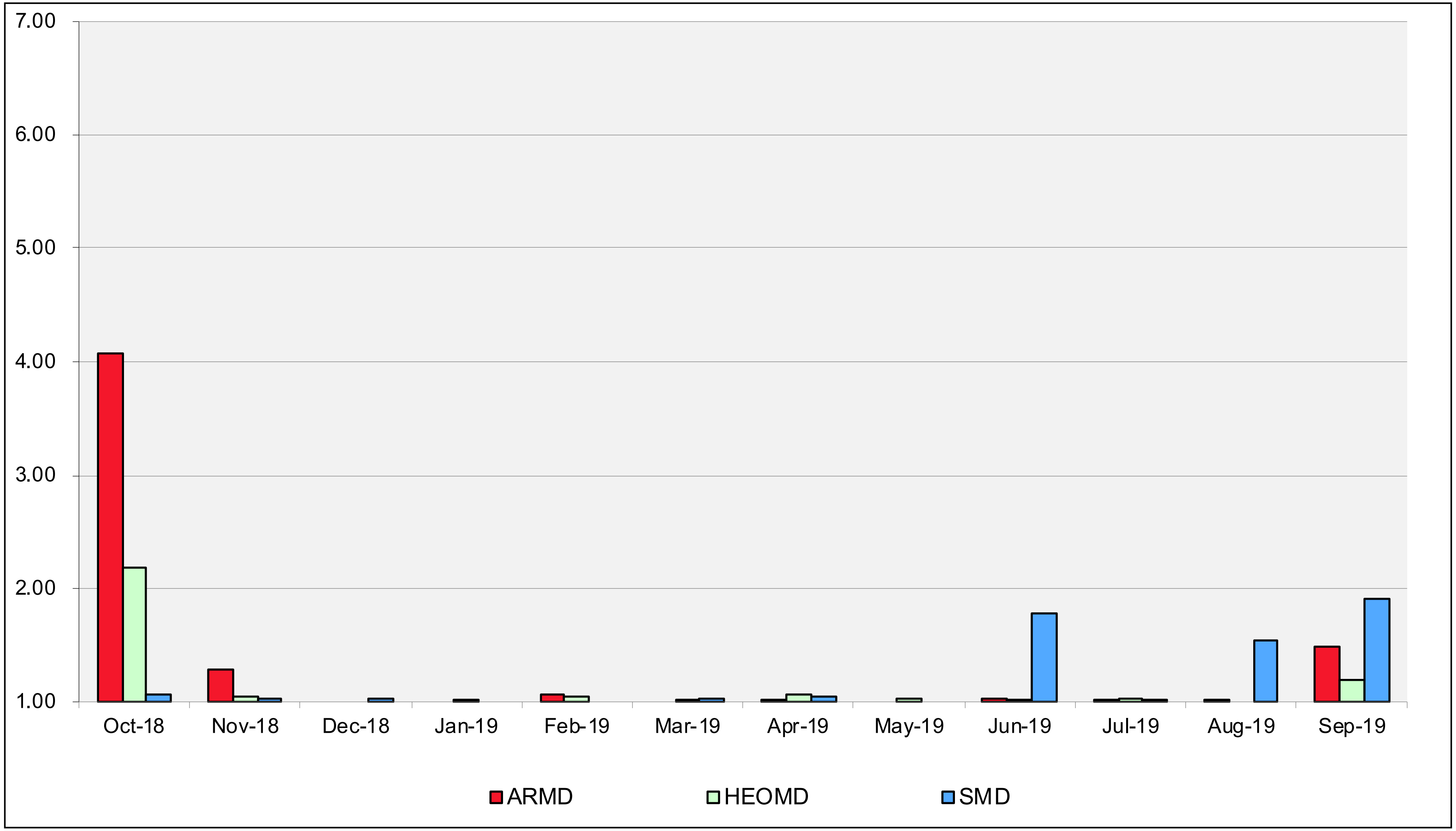
Merope: Monthly Utilization by Size and Length



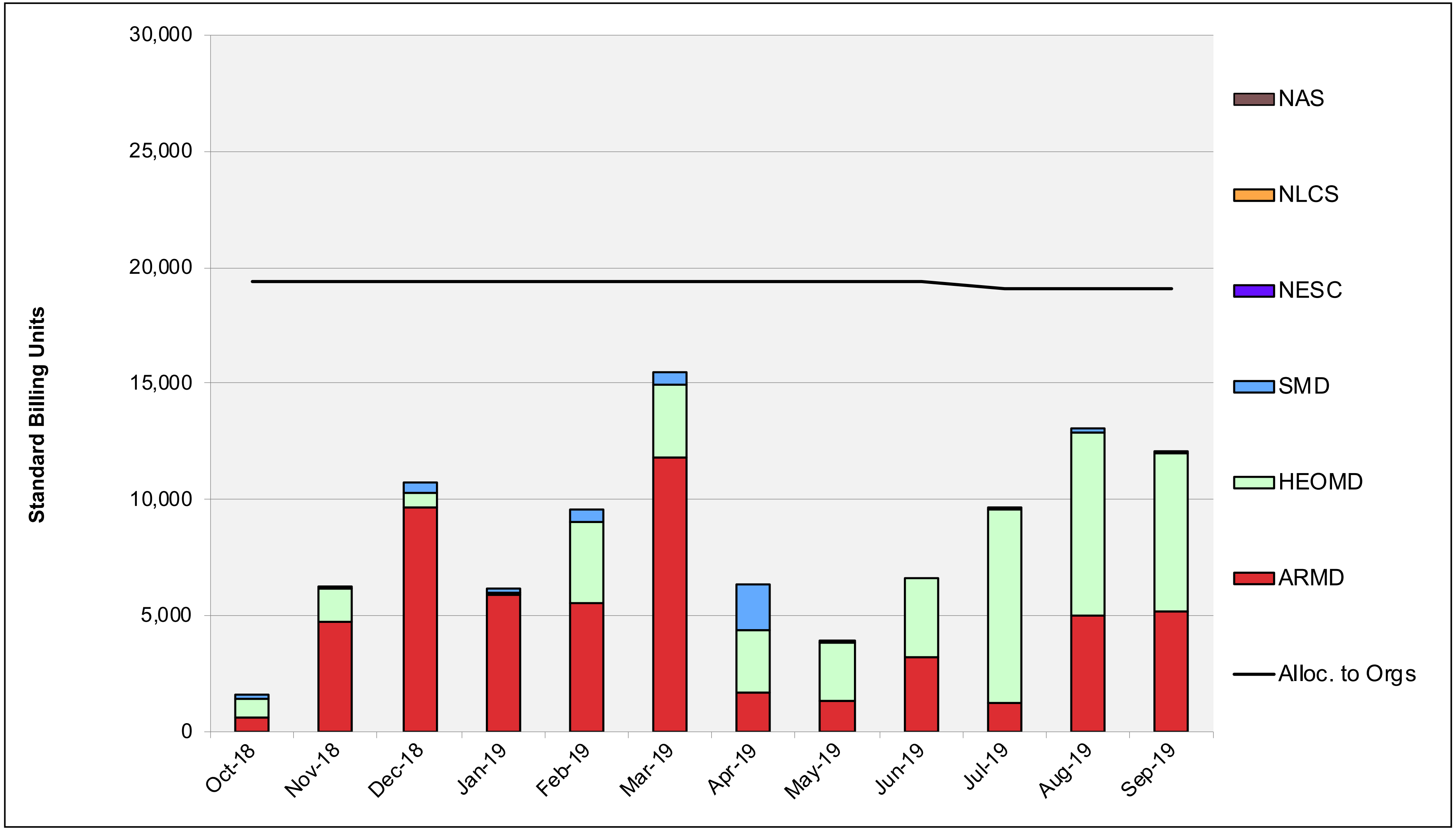
Merope: Average Time to Clear All Jobs



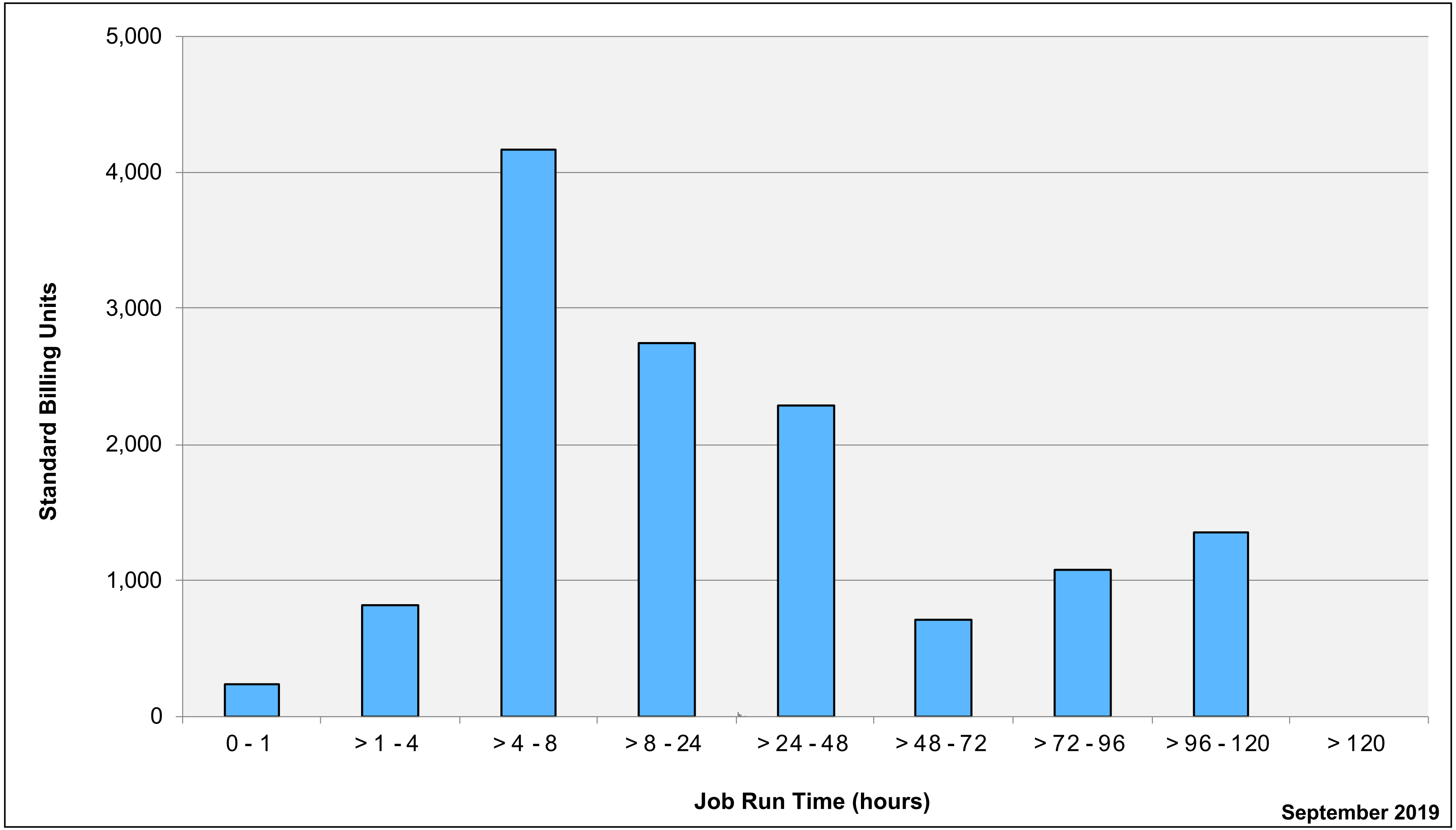
Merope: Average Expansion Factor



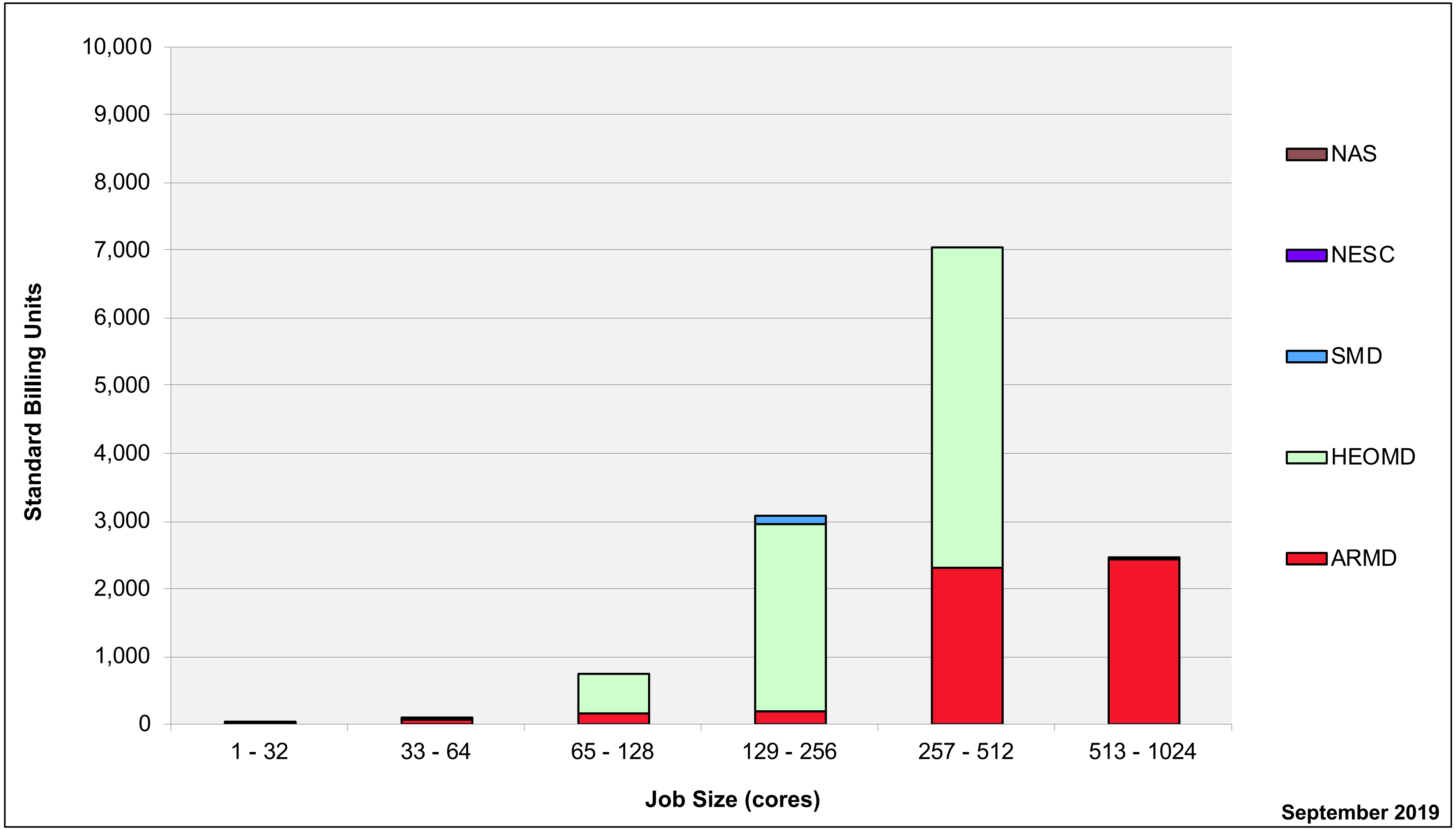
Endeavour: SBUs Reported, Normalized to 30-Day Month



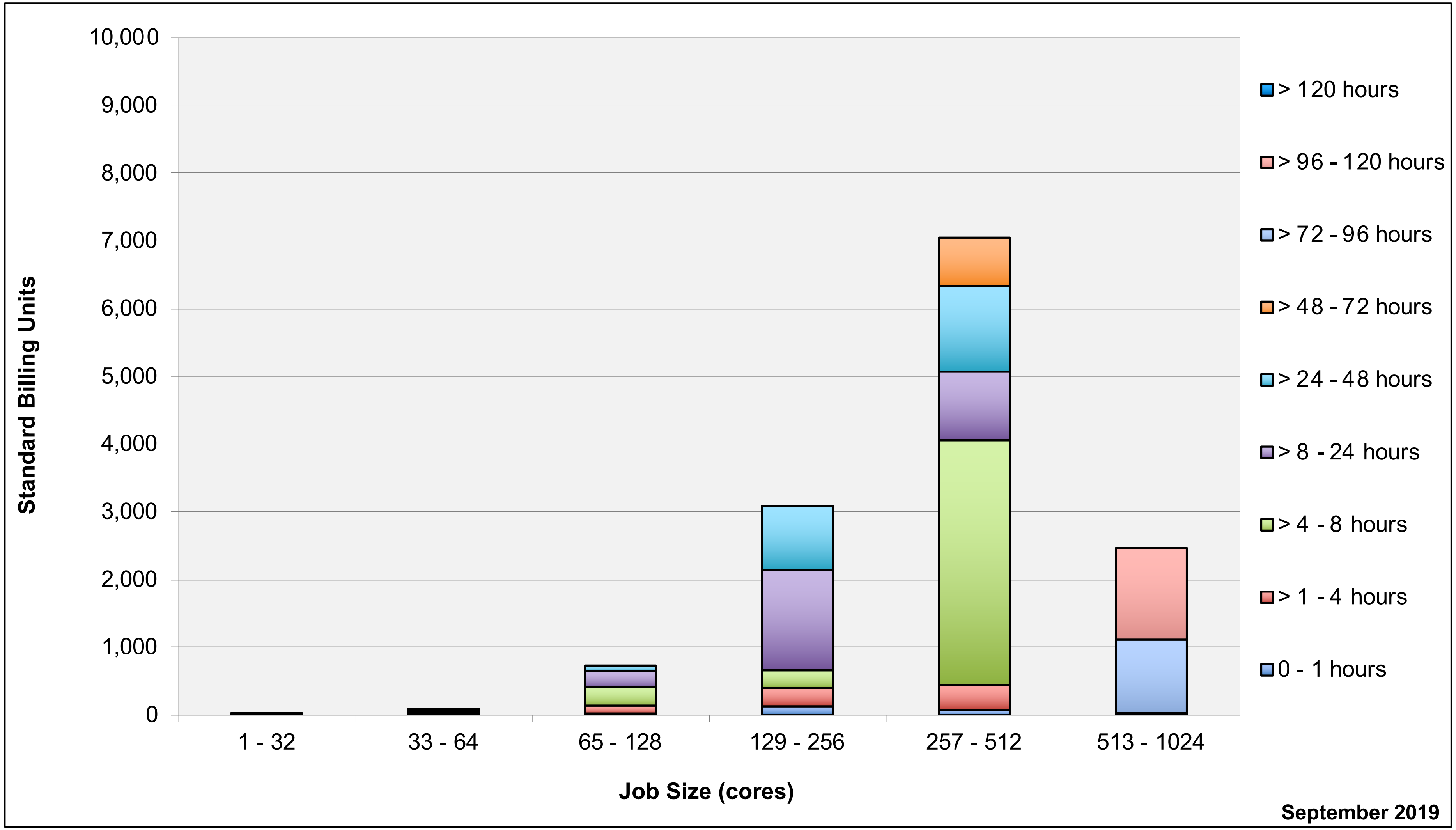
Endeavour: Monthly Utilization by Job Length



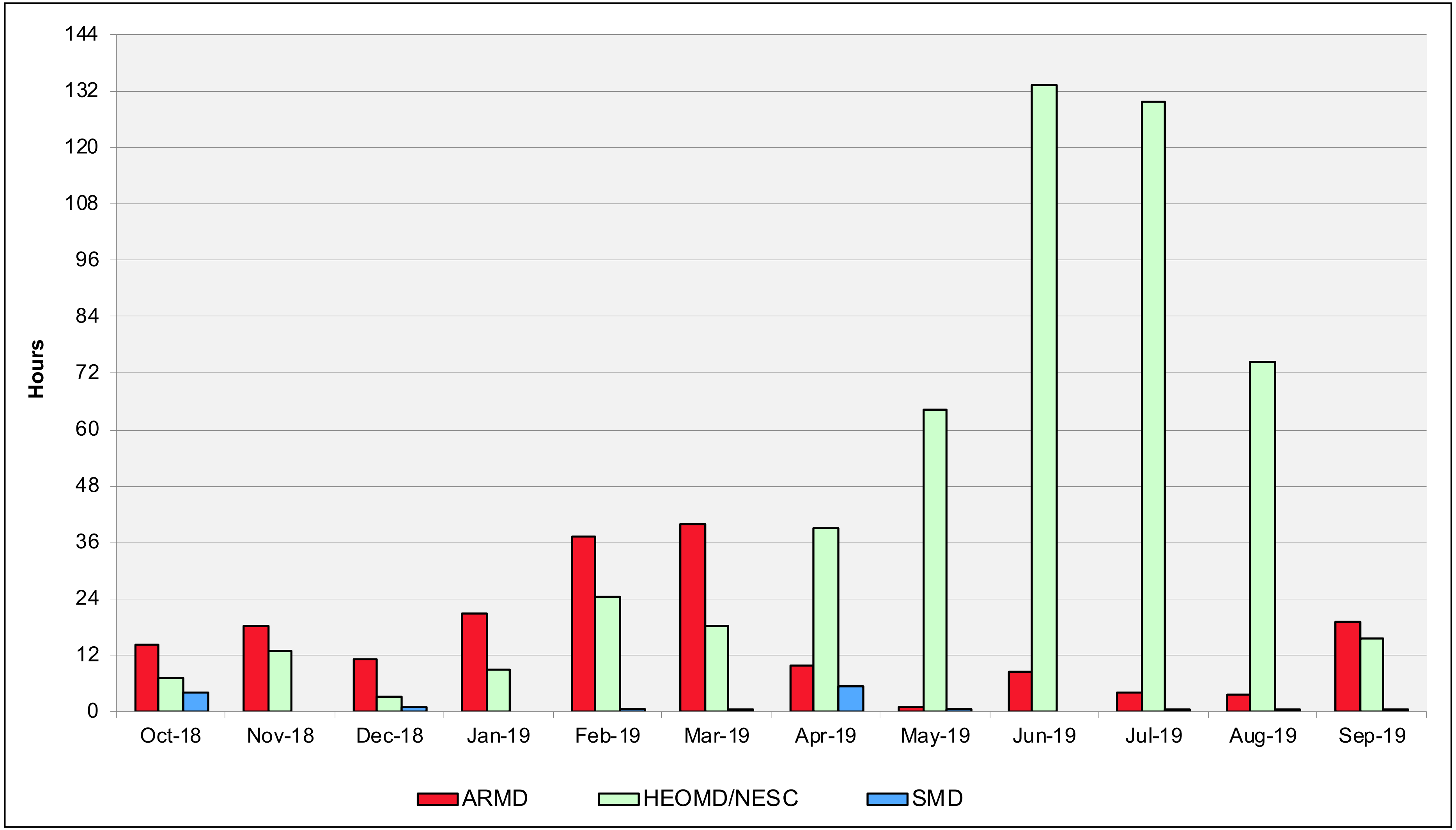
Endeavour: Monthly Utilization by Job Length



Endeavour: Monthly Utilization by Size and Length



Endeavour: Average Time to Clear All Jobs



Endeavour: Average Expansion Factor