Project Status Report

High End Computing Capability

Strategic Capabilities Assets Program

May 10, 2018

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NAS Facility Expansion (NFE) Project is Now in Full Swing

- The HECC Facilities team, in collaboration with Ames Code J and vendors Jacobs, Tri-Technic, HPE, and Schneider Electric, worked towards the November 2018 completion date of the NFE site. Activities this month included:
- Generated critical environmental documents and completed tests with county and state approvals, allowing ground work tasks to begin.
  - Key to starting the ground work was the removal of seven condemned trailers with asbestos abatement, and relocation of existing utilities running through the site.
  - Aggregate base is being delivered, leveled, and compacted to raise the one-acre site as much as 60 inches to mitigate possible future sea level rise.
- Module designers HPE and Schneider delivered their 30% design package and are nearing 60% design completion.
- Placed purchase orders for long-lead items (30 megawatt transformer, 115 kilovolt breaker).
- Continued planning for duct-bank construction and module design completion (through June).

Mission Impact: The NFE design builds on the enormous success of HECC's prototype Modular Supercomputing Facility, which has proven to be a much more cost-effective and energy-efficient way to operate and manage a supercomputing environment.

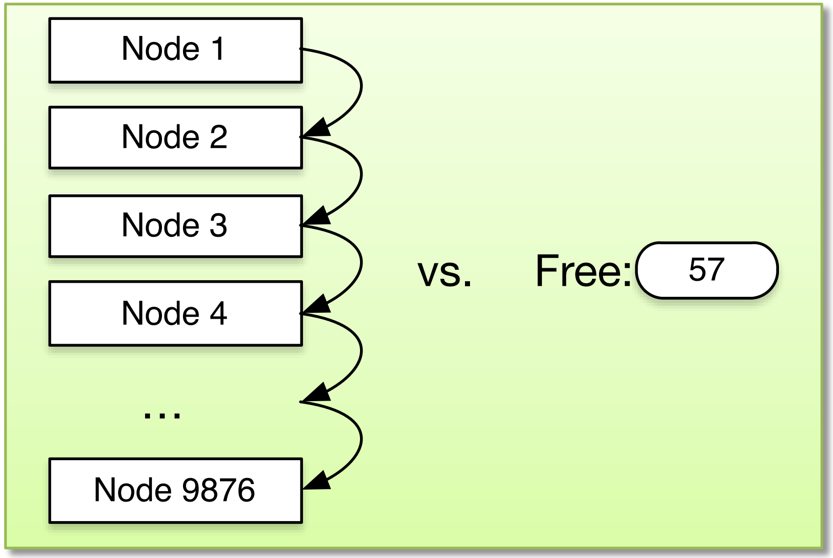
Ground work is underway on the one-acre construction site that will house the NAS Facility Expansion. Once completed, the site will distribute nearly 30 megawatts of power to up to 16 modular buildings housing high-end computing and storage resources.

POCs: William Thigpen, william.w.thigpen@nasa.gov, (650) 604-1061, NASA Advanced Supercomputing (NAS) Division; Chris Tanner, christopher.tanner@nasa.gov, (650) 604-6754, NAS Division, CSRA LLC

Production PBSPro Job Scheduler Improved with HECC Staff Designed Algorithm

- HECC Supercomputing Systems staff designed a job scheduling algorithm that was put into production use by PBSPro vendor Altair.
- The production scheduler performs four times faster than the previous version, and forecasts the start time of 50% more high-priority jobs.
- Increased scheduler performance improves utilization on Pleiades and Electra by quickly starting jobs on available nodes. Job forecasting is critical to ensure resources will be made available as soon as possible for high-priority requests.
- The improved scheduler enables the design and use of additional features that are otherwise too computationally expensive.
- HECC staff are working with Altair to design a feature allowing users to request compute nodes in a more flexible manner.

Mission Impact: An in-house algorithm designed for scheduling work done on HECC supercomputers increases scheduling performance and improves the utilization of NASA's computational resources.



HECC's job scheduling algorithm eliminates repeated expensive searches through lists of nodes by aggregating information in advance and adjusting the count of nodes when scheduling jobs. This method performs very well on large clusters like Pleiades and Electra with hundreds of identical nodes.

POCs: Greg Matthews, gregory.a.matthews@nasa.gov (650) 604-1321, and Dale Talcott, dale.r.talcott@nasa.gov, (650) 604-0555, NASA Advanced Supercomputing Division, CSRA LLC

Applications Team Uses Power Usage Data to Improve System Productivity

- HECC's Application Performance and Productivity (APP) team helped several users achieve significant improvements when their jobs exhibited symptoms of load imbalance.
- The team used their energy usage framework (see January 2018 report) to identify jobs showing a mismatch between power consumed on the two processor chips on each node—typically caused by leaving a different number of cores idle on each.
- Balancing the work can lead to significant performance improvements for users:
  - One user reported an 11% reduction in SBU usage through using all 24 cores on a Haswell node rather than only 16 cores in an unbalanced fashion.
  - A novice user saw a 70% improvement when he started using all of the cores on a Broadwell node.
  - Another user saw a 3x improvement in an application using pthreads when he overrode the very inefficient default thread binding scheme.
  - A user with a hybrid MPI-OpenMP code saw a 4x speedup once threads were bound properly to cores.
- In the future, the APP group will use the energy framework to identify other types of inefficiencies in resource utilization.

Mission Impact: By load balancing compute jobs, HECC experts ensure that users get the same scientific or engineering work done using less time on supercomputing resources. This improves system productivity—time saved can be applied to other work.

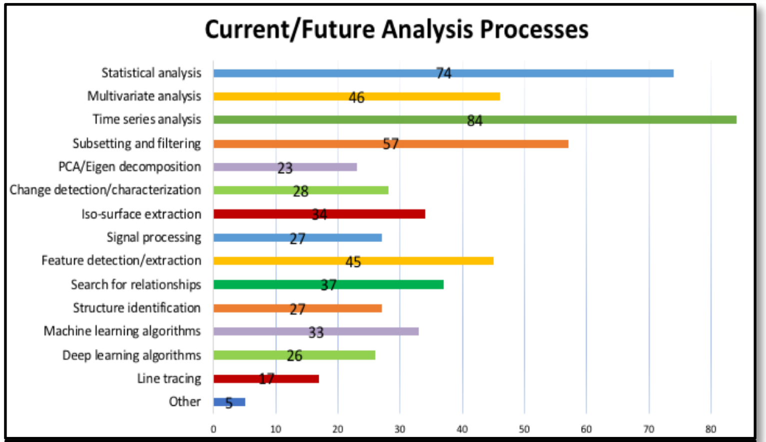
HECC's Application Performance and Productivity team measures the energy consumption of jobs running on the Pleiades and Electra systems, and identifies those exhibiting an imbalance of work done by each core. They then work with users to fix the issues leading to the imbalance.

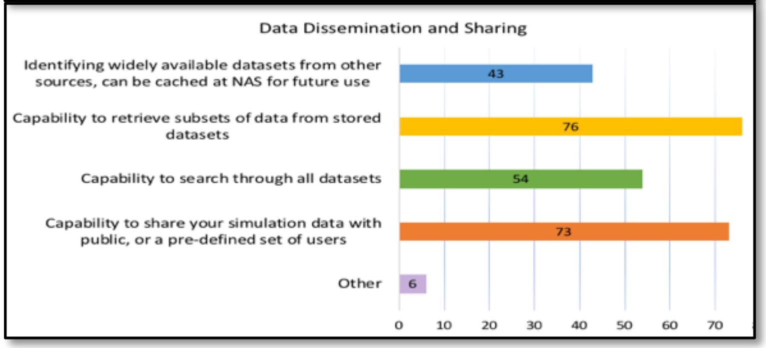
POCs: Robert Hood, robert.hood@nasa.gov, (650) 604-0740, NASA Advanced Supercomputing (NAS) Division, and Sherry Chang, sherry.chang@nasa.gov, (650) 604-1272, NAS Division, CSRA LLC

Big Data Survey Gathers User Feedback on Data Sharing and Data Analytics

- The HECC Big Data team completed the results of a survey sent to users from all mission directorates, academia, and industry, plus members of the Big Data Working Group.
- The survey received 191 responses; 35 users provided contact details for follow-up discussions.
  - Users provided feedback on their issues with data access, handling, and data sharing.
  - In addition to data management, users gave insight into requested capabilities that would increase their productivity in advanced analytics.
- Key areas of enhancements requested by users (see graphs at right):
  - Graphics processing unit (GPU) cluster expansion/ upgrade, big data platforms, sharable workflows.
  - Proposal to cache and store commonly used datasets in the HECC environment.
  - Provide mechanisms for data discovery, data sub-setting, and sharing data with other NASA and non-NASA users.
  - Assistance for moving into advanced analytics, and data analytics capabilities.
- The results of the survey will be utilized to plan for augmenting future platforms and services.

Mission Impact: The Big Data Survey helps determine the future needs of HECC's user community in the areas of data sharing, data analytics and machine learning/artificial intelligence infrastructure services for NASA missions.





POC: Shubha Ranjan, shubha.ranjan@nasa.gov, (650) 604-1918, NASA Advanced Supercomputing Division

Interactive Video Jukebox Developed for Supporting Live Events

- The HECC Tools team developed an interactive video jukebox application for use at conferences, tours, and other live events. The app debuted at the recent Silicon Valley Comic Con, where staff used it to showcase NASA science and engineering advances enabled by HECC resources (slide 8).
- The interactive video jukebox, coded in HTML, CSS, and Javascript, can be run in a browser over the internet or entirely from a local disk (as backup in case onsite network connections are unreliable). The app is controlled from an attached or wireless keyboard.
- Presenters can select/pause/play videos using the arrow keys and spacebar while explaining the details of simulations or responding to questions from the audience. In the absence of presenter interaction, the videos will play in a continuous loop.
- Action keys can also be customized to trigger popup screens showing URLs or QR codes that link to additional information on specific topics.

Mission Impact: The Interactive Video Jukebox app is an eye-catching, flexible, and easy-to-use tool for highlighting HECC services and user successes during live events.

Screenshot showing the interactive video jukebox interface with five featured videos loaded. Videos can easily be changed for different events. The video accompanying this slide shows in sequence: Normal operation, selecting and playing a different featured video, pausing the video, bringing up additional information with an action key, and starting the video again.

POC: John Hardman, john.hardman@nasa.gov, (650) 604-0417, NASA Advanced Supercomputing Division, CSRA LLC

NASA's Supercomputing Superheroes Shine at Silicon Valley Comic Con

- In an exciting sequel to last year's event, a team of HECC researchers and support staff produced its second successful outreach exhibit in the NASA booth at Silicon Valley Comic Con, held April 6–8 in San Jose, CA.
- The exhibit was featured as part of an extensive NASA presence at the event, which drew 65,000 people. HECC staff greeted thousands of attendees who were thrilled to talk to experts about the role of supercomputing and modeling & simulation in the agency's missions.
- An innovative video tool developed by the HECC Tools Team (see slide 7) made it possible to easily display compelling visualizations from research across all mission directorates.
- Simulations shared with visitors included predictions of the August 2017 total solar eclipse; atmospheric entry of meteoroids; complex quadcopter aerodynamics; and ascent abort scenarios for the Orion spacecraft's Launch Abort Vehicle.
- Aerospace engineer Derek Dalle, of the NASA Advanced Supercomputing Division, participated in the "NASA's Journey to Mars" panel, discussing the impact of HECC-enabled modeling and simulation on launch ascent vehicle development.

Mission Impact: NASA's exhibit at Silicon Valley Comic Con provided an excellent public outreach opportunity to highlight the critical role of HECC resources in science and engineering projects across the agency.

Top: HECC Deputy Project Manager Bill Thigpen (left) shares a laugh with security expert Bond Nguyen. *Blaise Hartman, NASA/Ames*

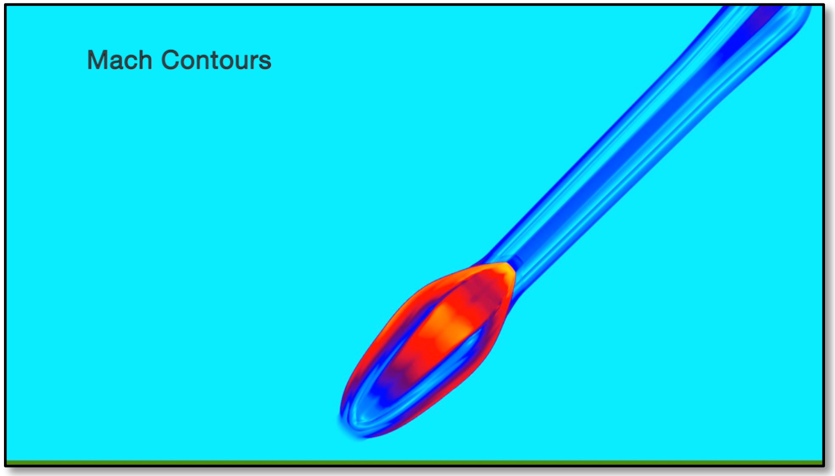
Bottom: The HECC exhibit attracted thousands of SVCC attendees. *Derek Shaw, NASA/Ames*

POC: Michelle Moyer, michelle.c.moyer@nasa.gov, (650) 604 2912, NASA Advanced Supercomputing Division, CSRA LLC

Simulating Atmospheric Airbursts of Pebble- to Mountain-Size Meteoroids*

- Researchers at NASA Ames ran new, high-fidelity simulations of centimeter- to kilometer-size meteoroids on Pleiades and Endeavour to accurately predict ground overpressures and wind speeds generated by meteoric airbursts.
- The researchers coupled the capabilities of NASA's Cart3D software with an atmospheric propagation solver to handle the propagation of weaker pressure disturbances from small, fist-size meteoroids. Results are used to:
  – Verify luminous, ionization, and acoustic efficiencies to improve meteoroid mass estimates.
  – Help calibrate optical and infrasound observations.
- A detailed reconstruction of the 2013 Chelyabinsk event produced excellent agreement between the simulation and actual recorded arrival times and ground overpressures.
- The large capacity of Pleiades is critical for handling the numerous uncertainties associated with atmospheric impacts of meteoroids.

Mission Impact: These high-fidelity simulations, enabled by the Pleiades supercomputer, are being used to create improved damage and risk models for the Asteroid Threat Assessment Project within NASA's Planetary Defense Coordination Office.



Video from a simulation of an airburst at an altitude of about 10 kilometers (km) from a meteoroid with an entry speed of 20 km/s and a diameter of 60 meters. The energy release is equivalent to 10 megatons of TNT. *Michael Aftosmis, Marian Nemec, NASA/Ames*

POCs: Marian Nemec, marian.nemec@nasa.gov, (650) 604-4319, Michael Aftosmis, (650) 604-4499, NASA Advanced Supercomputing Division

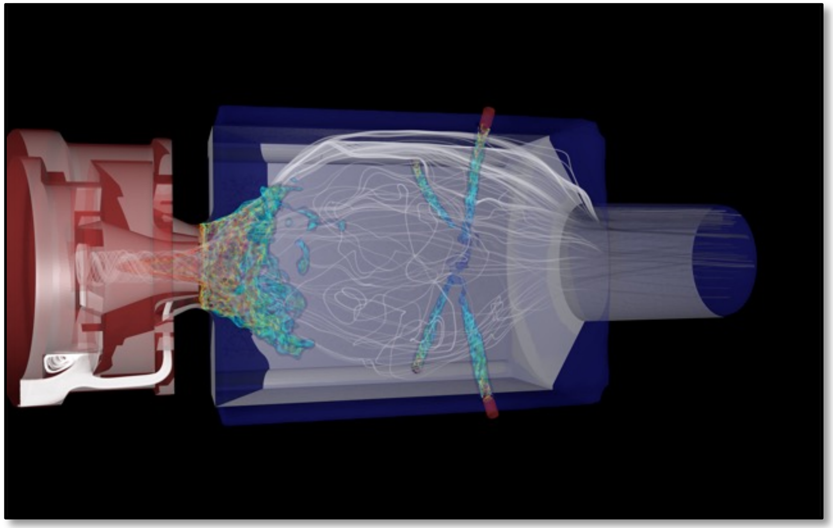
**HECC provided supercomputing resources and services in support of this work.*

Researchers Simulate How Soot Forms in Jet Engines, Aiming to Reduce Emissions*

- University of Michigan researchers ran simulations on Pleiades to help answer fundamental questions about how soot forms in jet engines, coagulates, and grows to large agglomerate structures.
- Results led to the development of a validated reacting flow model that is coupled to soot particle dynamics.
  - Analysis showed how recirculation zones within the combustor help stabilize the flame and reduce soot.
  - Researchers identified different types of particle trajectories that indicated the timescale of soot formation and oxidation.
  - The end result: soot is reduced via dilution jet injection, which enhances the strength of the inner recirculation zone.
- The long-term goal is to understand how to use aerodynamic straining to oxidize soot particles before they grow into larger particles, eventually helping to reduce soot emissions.

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

Mission Impact: Modeling and simulation on HECC resources enabled researchers to understand reasons why soot forms in jet engines, and simulate ways to reduce it—helping engineers to eventually design cleaner, more efficient engines.



High-velocity, swirling air streams (multicolored contours) are injected into a simulated jet engine to enhance mixing and guide the flame. Secondary air jets are injected at a downstream location to dilute the post-combustion mixture and reduce soot formation. Recirculation in the center of the combustor, shown by the flow streamlines (white lines), is also critical to flame stabilization and soot reduction.

POCs: Alex Chong, stchong@umich.edu, and Venkat Raman, ramanvr@umich.edu, (734) 764-4318, Advanced Propulsion Concepts Lab, University of Michigan

HECC Facility Hosts Several Visitors and Tours in April 2018

- HECC hosted 14 tour groups in April; 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:
  - Sir Roger Penrose, the famous English mathematical physicist, mathematician, and philosopher of science. He is a Emeritus Rouse Ball Professor of Mathematics in the University of Oxford and Emeritus Fellow of Wadham College, Oxford.
  - Rick Snyder, Governor of Michigan.
  - His Excellency Pema Khandu, Chief Minister of Arunachal Pradesh, Republic of India.
  - Frank Indiviglio, Acting Deputy Director High Performance Computing and Communication, National Oceanic and Atmospheric Administration.
  - A group from the Australian Ministry of Law Enforcement.
  - Students from the University College of London, who are in their first year of a four-year doctoral program in quantum technologies.
  - National Defense University (Eisenhower School), Information and Communications Technology Industry Study Group.

Piyush Mehrotra, Chief, NASA Advanced Supercomputing Division, gave a hyperwall presentation to Michigan Governor Rick Synder.

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

Papers

- "**Solar Wind Interaction with the Martian Upper Atmosphere: Roles of the Variable 3D Cold Thermosphere and Hot Oxygen Corona**," C. Dong, et al., arXiv:1804.00937 [astro-ph.EP], April 3, 2018. *
  https://arxiv.org/abs/1804.00937
- "**A Continent-Wide Search for Antarctic Petrel Breeding Sites with Satellite Remote Sensing**," M. Schwaller, et al., Remote Sensing of Environment, Vol. 210, April 3, 2018. *
  https://www.sciencedirect.com/science/article/pii/S003442571830083X
- "**Dynamics of Trees of Fragmenting Granules in the Quiet Sun: Hinode/SOT Observations Compared to Numerical Simulation**," J. Malherbe, T. Roudier, R. Stein, Z. Frank, arXiv:1804.01870 [astro-ph.SR], April 5, 2018. *
  https://arxiv.org/abs/1804.01870
- "**Investing the Response of Loop Plasma to Nanoflare Heating Using RADYN Simulations**," V. Polito, et al., The Astrophysical Journal, Vol. 856, No. 2, April 5, 2018. *
  http://iopscience.iop.org/article/10.3847/1538-4357/aab49e/meta
- "**Smooth Sliding and Superlubricity in the Nanofriction of Collapsed Carbon Nanotubes**," H. Xu, J. Al-Ghalith, T. Dumitrica, Carbon (Elsevier), April 11, 2018. *
  https://www.sciencedirect.com/science/article/pii/S0008622318303567
- "**Hydrothermal Decomposition of Amino Acids and Origins of Prebiotic Meteoritic Organic Compounds**," F. Pietrucci, et al., ACS Earth Space Chemistry, April 11, 2018. *
  https://pubs.acs.org/doi/abs/10.1021/acsearthspacechem.8b00025
- "**Three-Dimensional Kinetic Pulsar Magnetosphere Models: Connecting to Gamma-Ray Observations**," C. Kalapotharakos, et al., The Astrophysical Journal, Vol. 857, No. 1, April 11, 2018. *
  http://iopscience.iop.org/article/10.3847/1538-4357/aab550/meta

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

Papers (cont.)

- **“Impact of Small-Scale Structures on Estuarine Circulation**,” Z. Liu, Y. Zhang, Ocean Dynamics, Vol. 68, Issue 4-5, April 14, 2018. *
  https://link.springer.com/article/10.1007%2Fs10236-018-1148-6
- “**Were Chondrites Magnetized by the Early Solar Wind?**” R. Oran, B. Weiss, O. Cohen, Earth and Planetary Science Letters, Vol. 492, April 17, 2018. *
  https://www.sciencedirect.com/science/article/pii/S0012821X1830075X
- **“Reiner Gamma Albedo Features Reproduced by Modeling Solar Wind Standoff**,” J. Deca, A. Divin, C. Lue, T. Ahmadi, M. Horanyi, Communications Physics, April 19, 2018. *
  https://www.nature.com/articles/s42005-018-0012-9
- “**Deep Learning Identifies High-z Galaxies in a Central Blue Nugget Phase in a Characteristic Mass Range**,” M. Huertas-Company, et al., arXiv:1804.07307 [astro-ph.GA], April 19, 2018. *
  https://arxiv.org/abs/1804.07307
- “**Is the Dark-Matter Halo Spin a Predictor of Galaxy Spin and Size?**” F. Jiang, et al., arXiv:1804.07306 [astro-ph.GA], April 19, 2018. *
  https://arxiv.org/abs/1804.07306
- “**Role of the Plasmoid Instability in Magnetrohydrodynamic Turbulence**,” C. Dong, et al., arXiv:1804.07361 [physics.plasm-ph], April 19, 2018*
  https://arxiv.org/abs/1804.07361
- “**Applying the Weighted Horizontal Magnetic Gradient Method to a Simulated Flaring Active Region**,” M. Korsos, P. Chatterjee, R. Erdelyi, The Astrophysical Journal, Vol. 857, No. 2, April 20, 2018. *
  http://iopscience.iop.org/article/10.3847/1538-4357/aab891/meta

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

Papers (cont.)

- "**Side-Jet Effects in High-Pressure Turbulent Flows: Direct Numerical Simulation of Nitrogen Injected into Carbon Dioxide**," A. Gnanaskandan, J. Bellan, The Journal of Supercritical Fluids, April 24, 2018. *
  https://www.sciencedirect.com/science/article/pii/S0896844617308926
- "**Tensor Calculus in Spherical Coordinates Using Jacobi Polynomials, Part II: Implementation and Examples**," D. Lecoanet, et al., arXiv:1804.09283 [astro-ph.IM], April 24, 2018. *
  https://arxiv.org/abs/1804.09283
- "**Kepler Data Validation I – Architecture, Diagnostic Tests, and Data Products for Vetting Transiting Planet Candidates**," J. Twicken, et al., Publications of the Astronomical Society of the Pacific, Vol. 130, No. 988, April 24, 2018. *
  http://iopscience.iop.org/article/10.1088/1538-3873/aab694
- "**Entrainment in Resolved, Turbulent Dry Thermals**," D. Lecoanet, N. Jeevanjee, arXiv:1804.09326 [physics.flu-dyn], April 25, 2018. *
  https://arxiv.org/abs/1804.09326
- "**Erratum: 'SIGAME Simulations of the [C $_{II}$], [O $_{I}$], and [O $_{III}$] Line Emission from Star-Forming Galaxies at z≃6' (2017, ApJ, 846, 105)**," K. Olsen, et al., The Astrophysical Journal, Vol. 857, No. 2, April 25, 2018. *
  http://iopscience.iop.org/article/10.3847/1538-4357/aabaf9/meta

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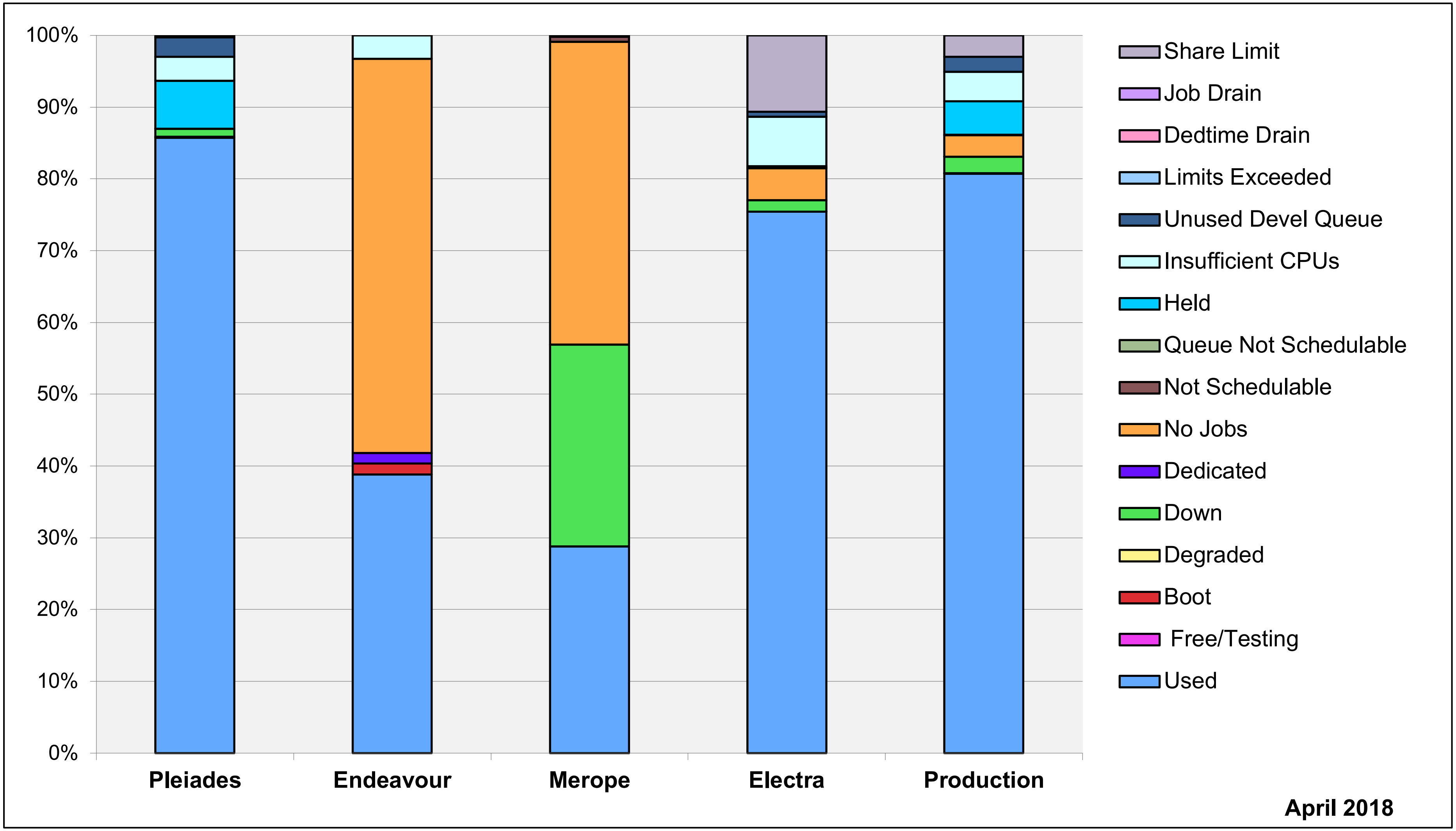
News and Events

- **Launch Abort! What Happens Next? NASA Scientists Figure Out of the Flow to Keep Astronauts Safe**, *NASA Ames Feature,* March 30, 2018—Research scientists at the NASA Advanced Supercomputing Division are producing highly detailed simulations and visualizations to help keep astronauts safe during the dynamic liftoff conditions of NASA's Orion spacecraft. (Based on original March 5, 2018 NAS feature story, "Helping Keep Astronauts Safe with Advanced Simulations, Visualization.") *https://www.nasa.gov/feature/ames/launch-abort-what-happens-next-nasa-scientists-figure-out-the-flow-to-keep-astronauts-safe*
  - **NASA Simulates Their Orion Abort System. Now That Would Be a Crazy Ride**, *Universe Today,* April 4, 2018. *https://www.universetoday.com/138933/nasa-simulates-their-orion-abort-system-now-that-would-be-a-crazy-ride/*
- **Transiting Exoplanet Survey Satellite (TESS) Science Data Pipeline**, *NASA Ames Press Release*, April 11, 2018—NASA's ongoing search for life in the universe produces a lot of data. The agency's new planet-hunting mission, TESS, will collect 27 gigabytes per day in its all-sky search for undiscovered planets and will require the processing power of NASA's Pleiades supercomputer. *https://www.nasa.gov/ames/tess-pipeline*
  - **NASA's Transiting Exoplanet Survey Satellite Heads for Final Science Orbit after Successful Launch**, *Sci News*, April 19, 2018. *http://www.sci-news.com/astronomy/nasa-tess-launch-05927.html*

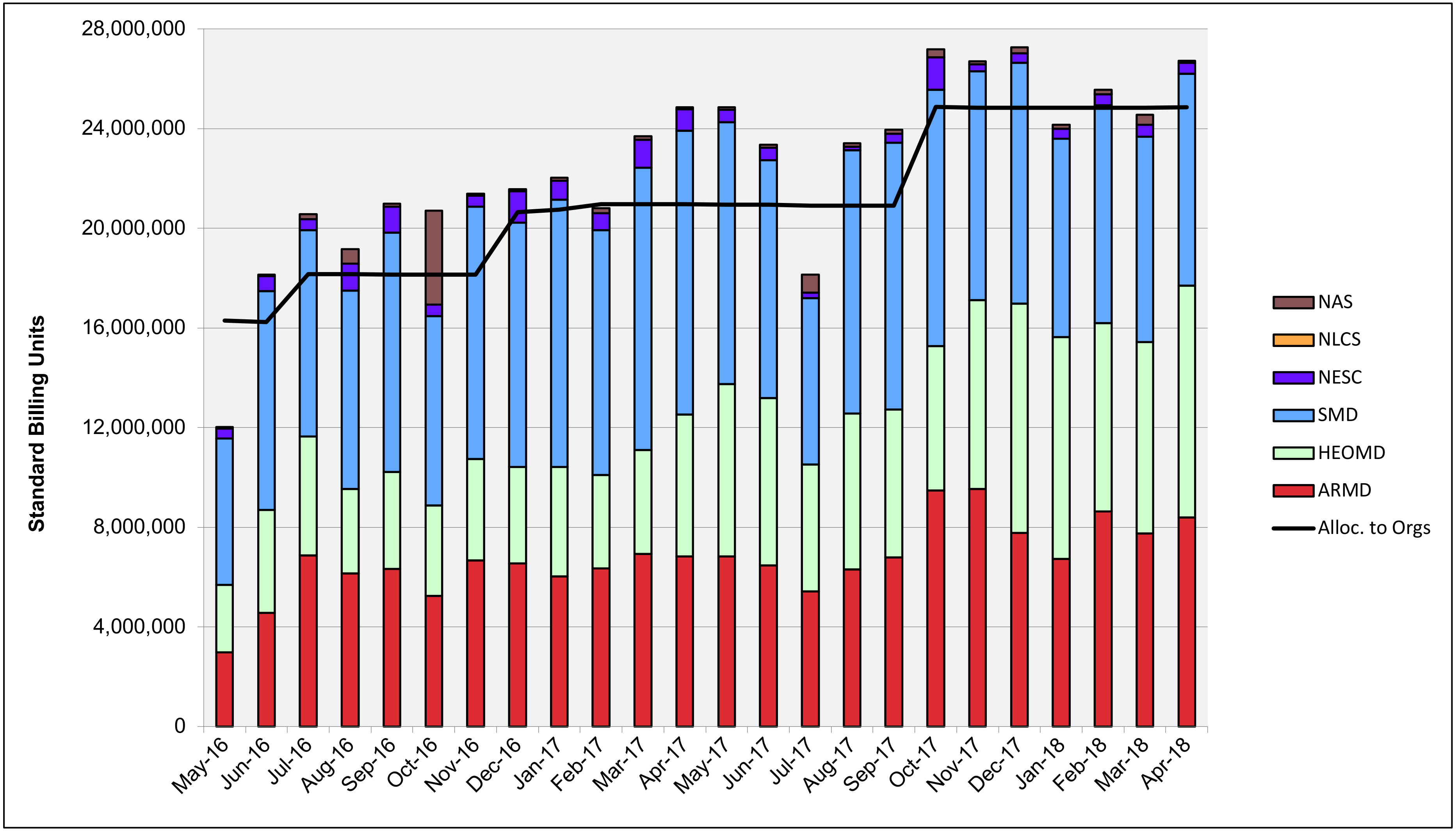
News and Events (cont.)

- **NASA Achieves Optimal Energy Efficiency with its First Modular Supercomputer**, *HPE Blog,* April 16, 2018—NASA has adopted a novel approach to cooling that not only enhances data center performance, but also conserves electricity and water. NASA's first modular supercomputer, Electra, is changing the game for researchers. *https://community.hpe.com/t5/Servers-The-Right-Compute/NASA-achieves-optimal-energy-efficiency-with-its-first-modular/ba-p/7002729#.WueijtPwZGF*
- **Lunar Swirl Features Reproduced by Modeling Solar Wind Standoff**, *SSERVI, Solar System Exploration Research Virtual Institute*, April 26 2018—Researchers at the Institute for Modeling Plasma, Atmospheres and Cosmic Dust (IMPACT) at the University of Colorado Boulder, used NASA's Pleiades supercomputer to develop the first 3D simulations to disentangle the movement of ions and electrons as the solar wind interacts with lunar magnetic anomalies. *https://sservi.nasa.gov/articles/lunar-swirl-features-reproduced-by-modeling-solar-wind-standoff/*

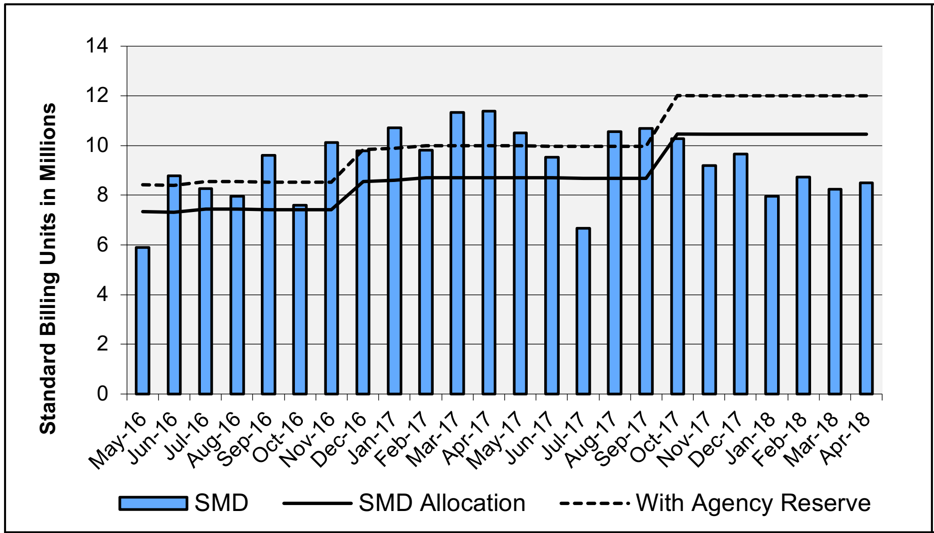
HECC Utilization

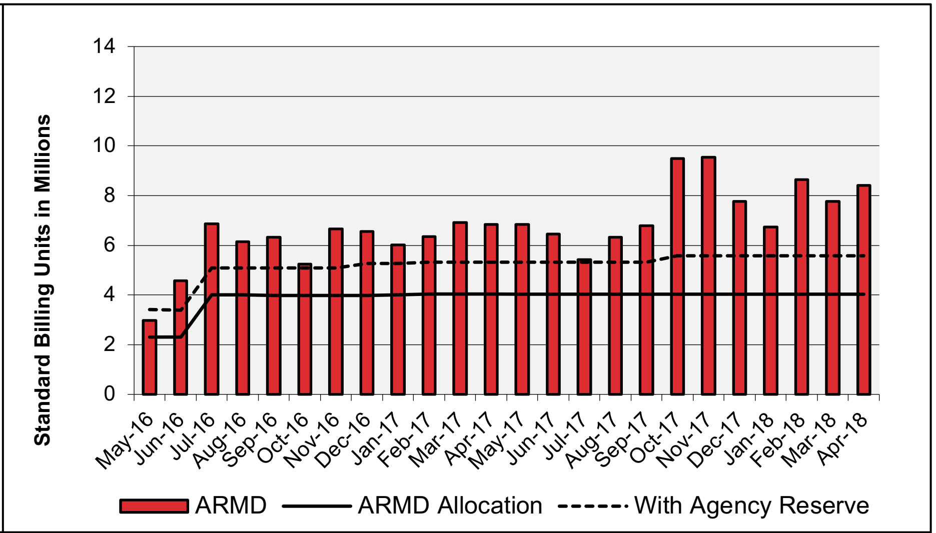


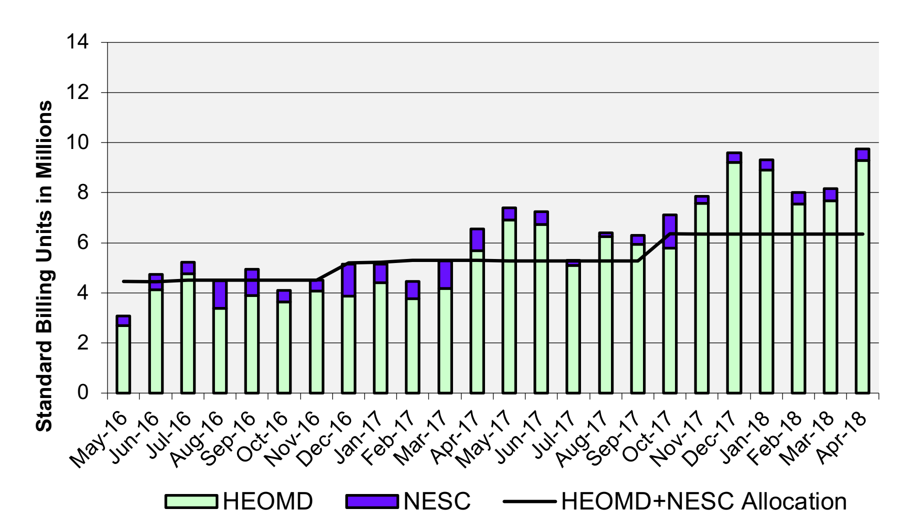
HECC Utilization Normalized to 30-Day Month



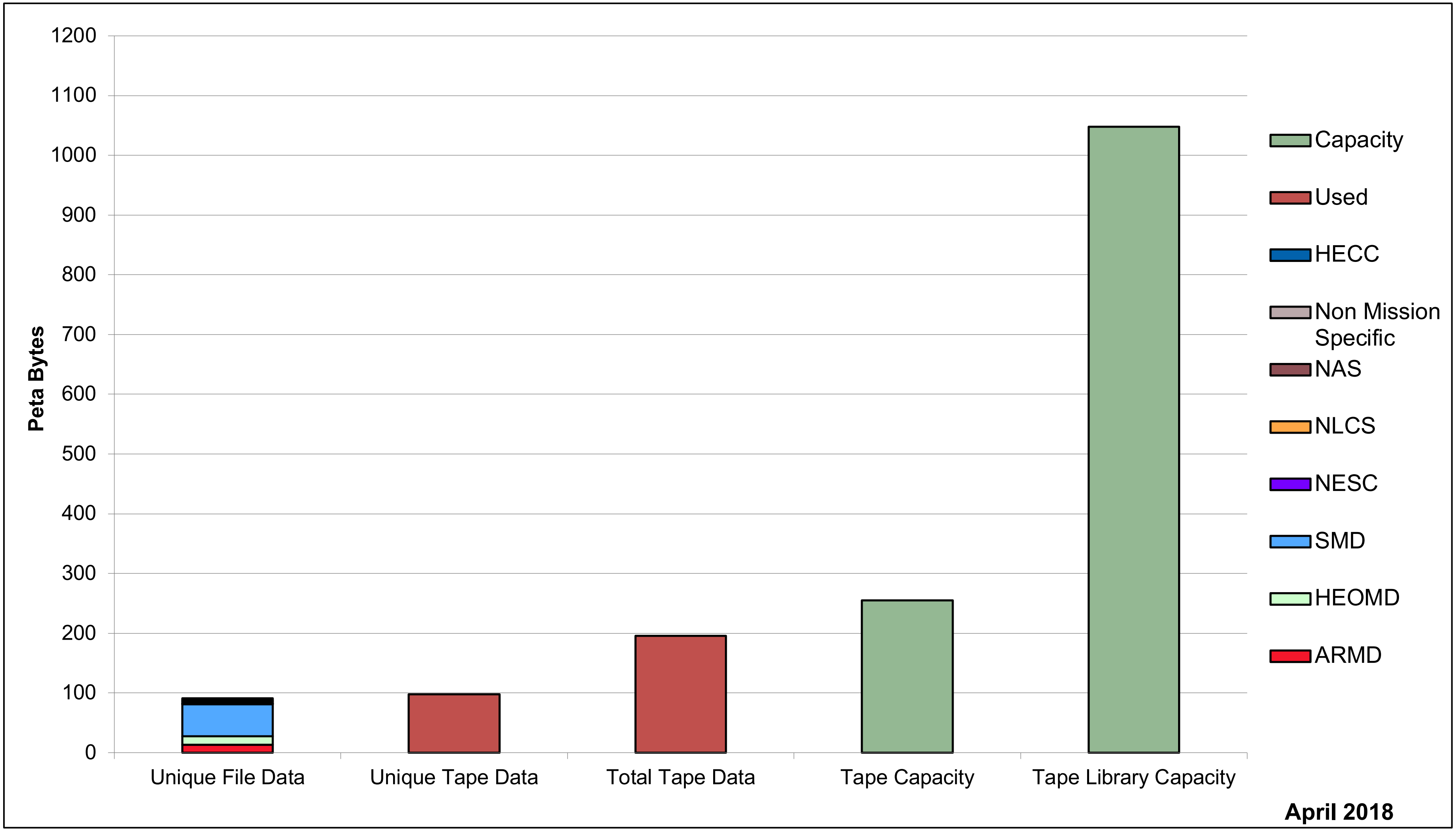
HECC Utilization Normalized to 30-Day Month







Tape Archive Status



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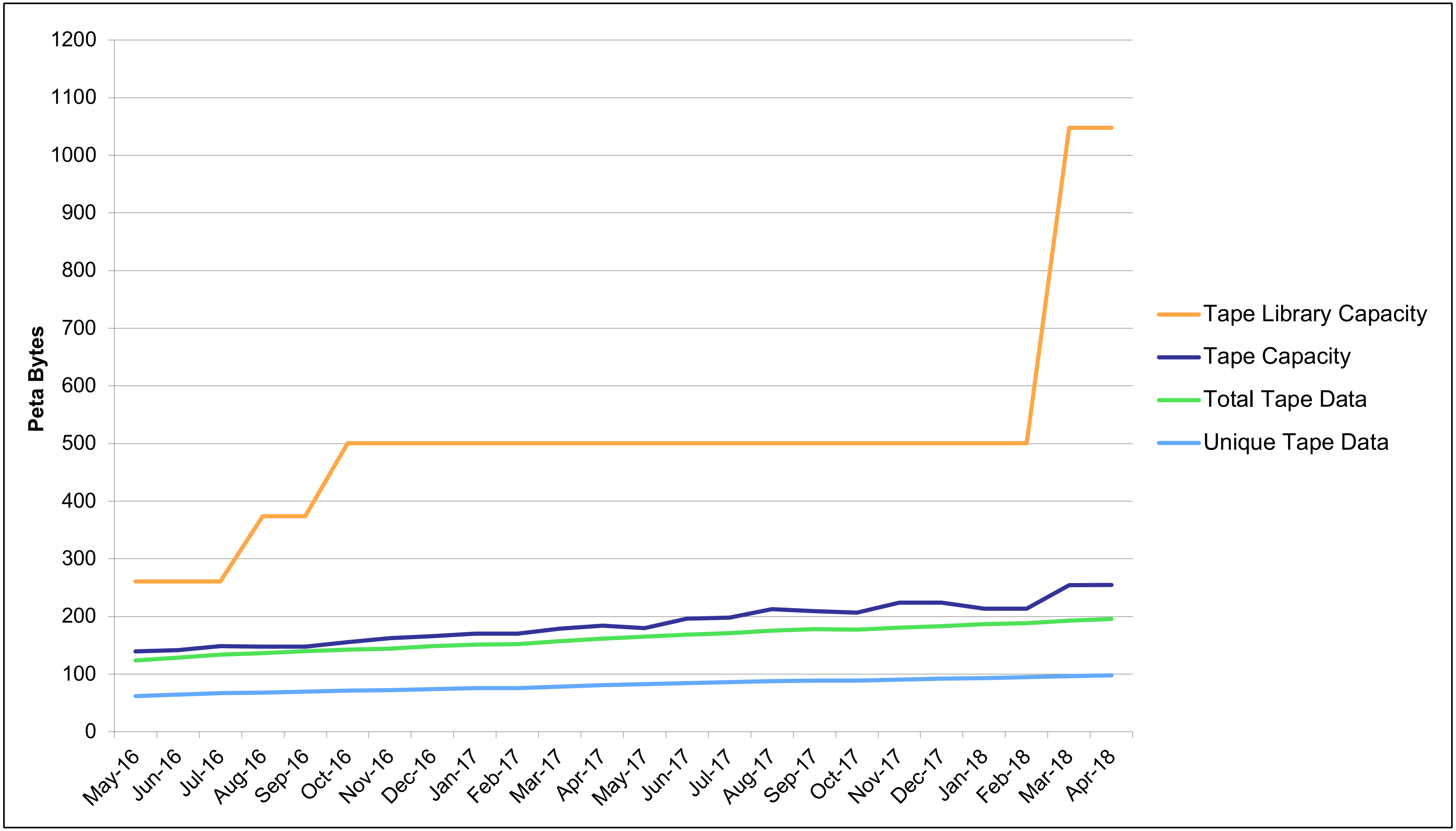
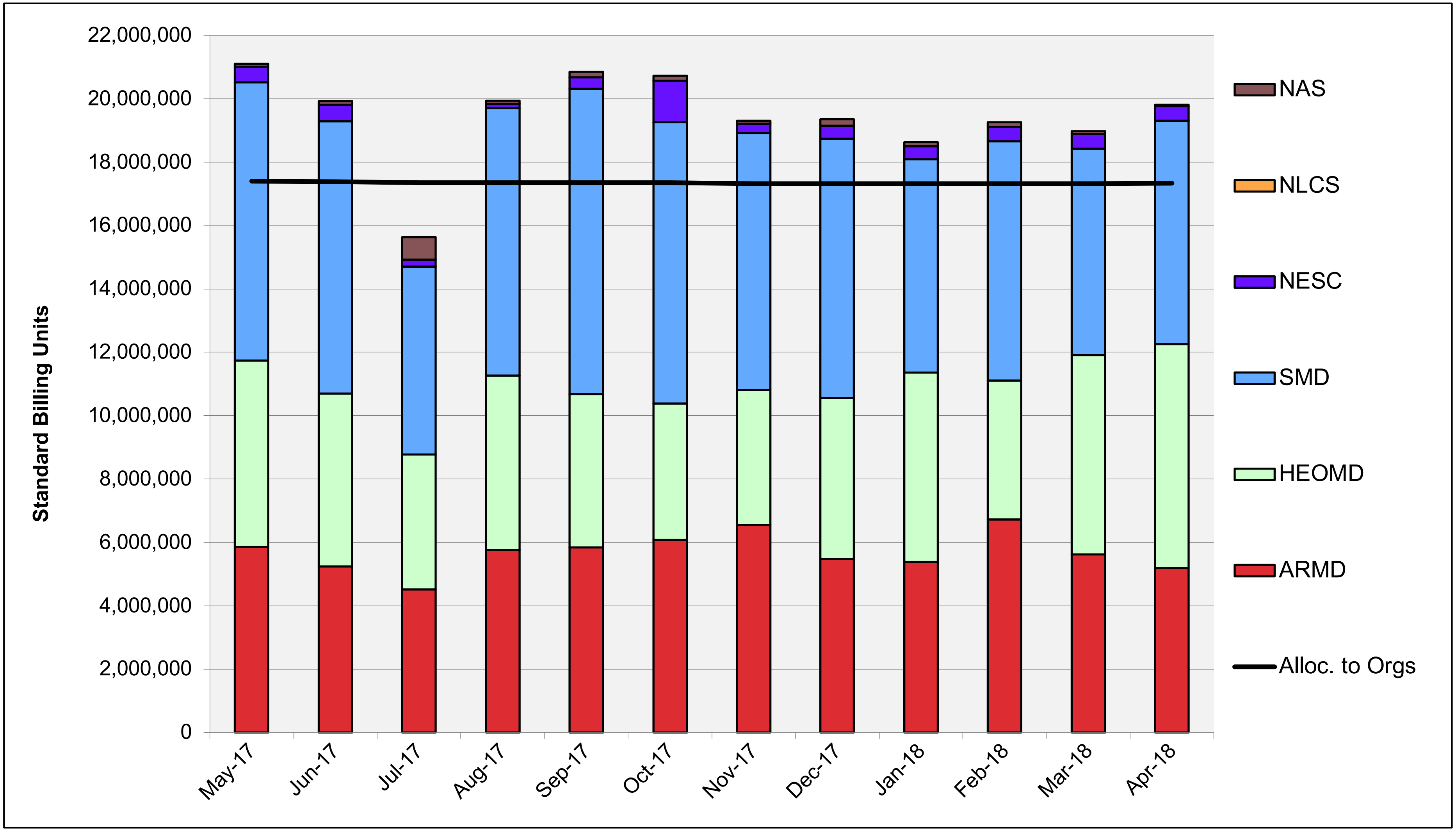
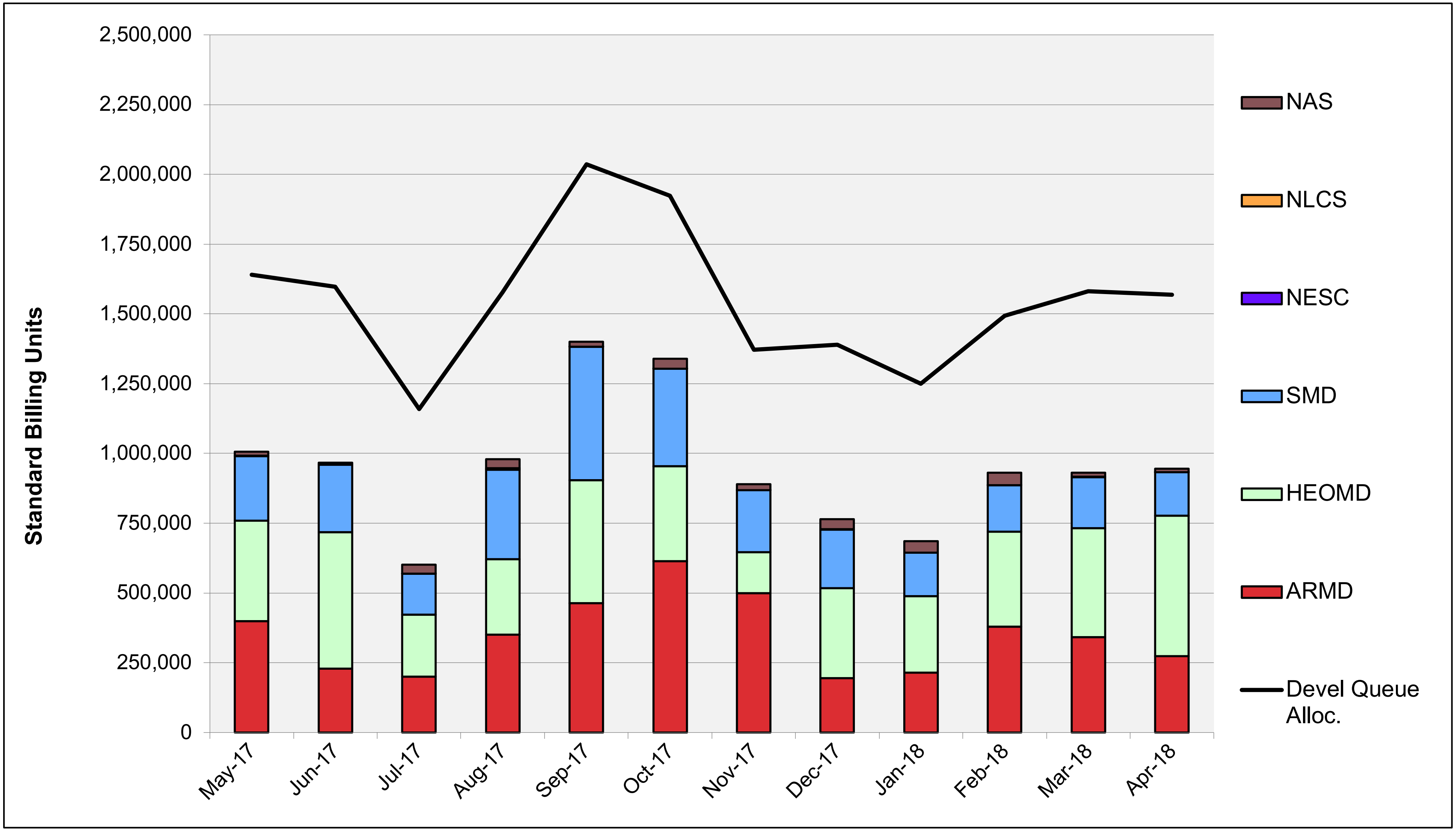


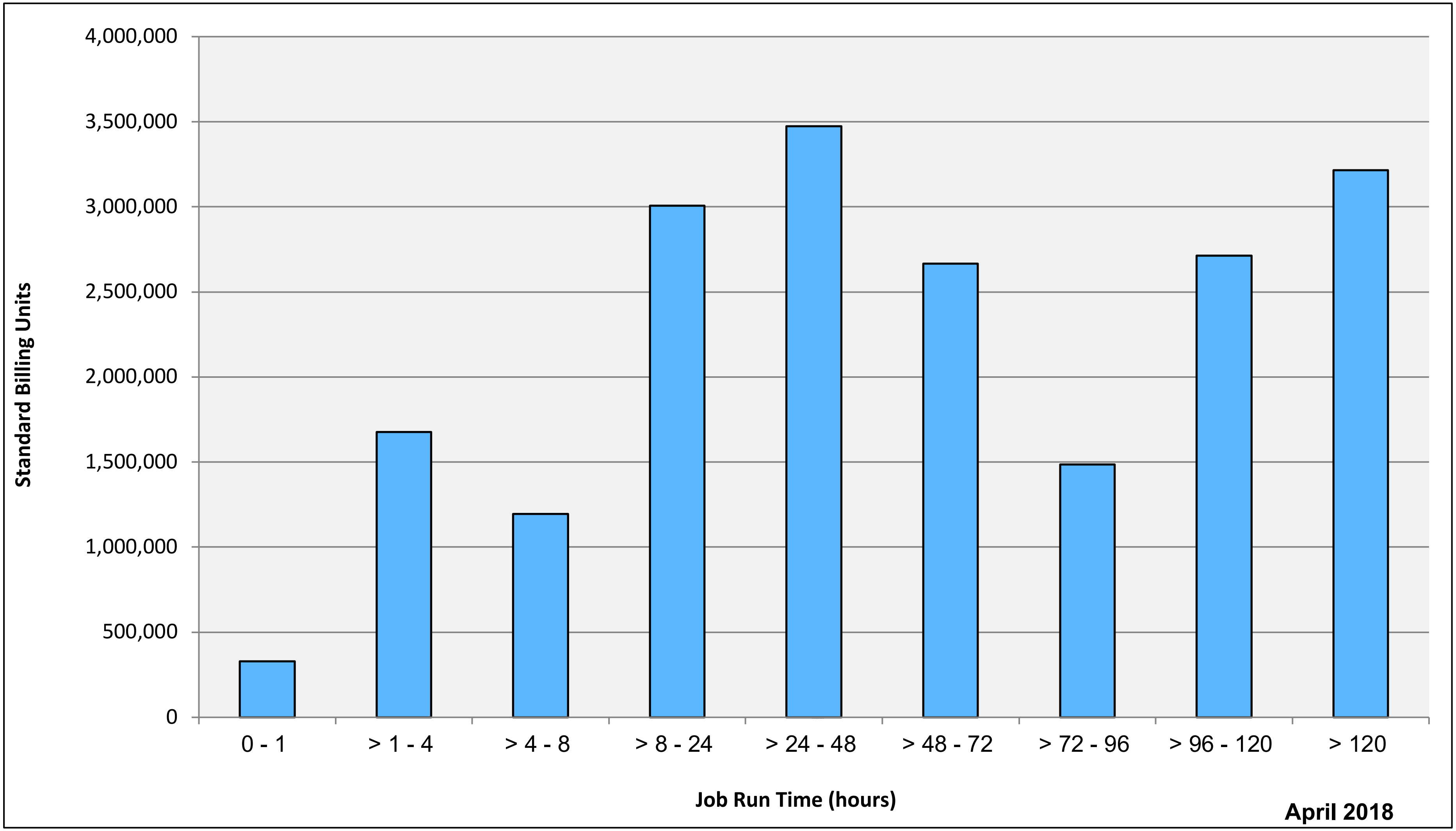
Pleiades: SBUs Reported, Normalized to 30-Day Month



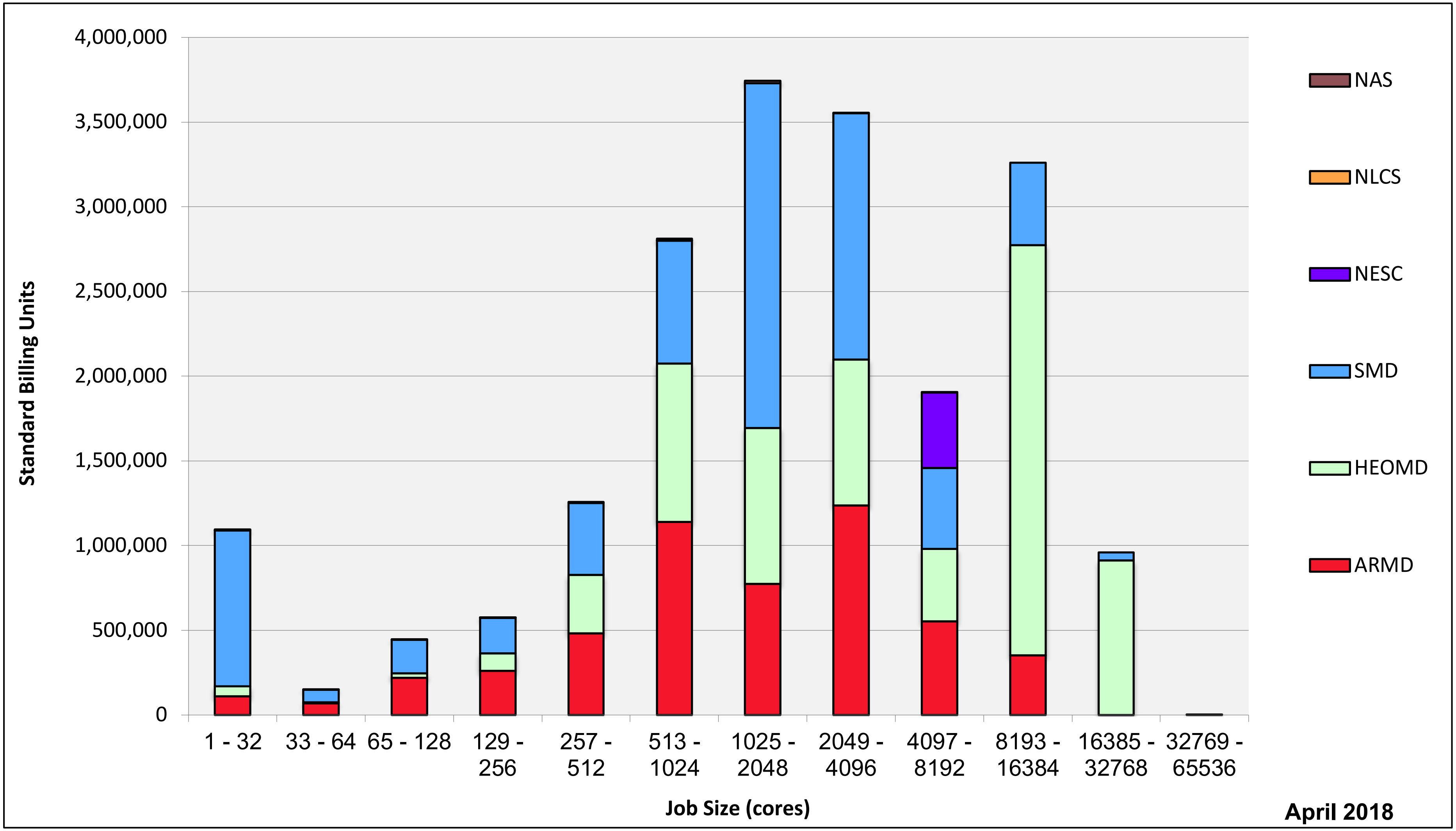
Pleiades: Devel Queue Utilization



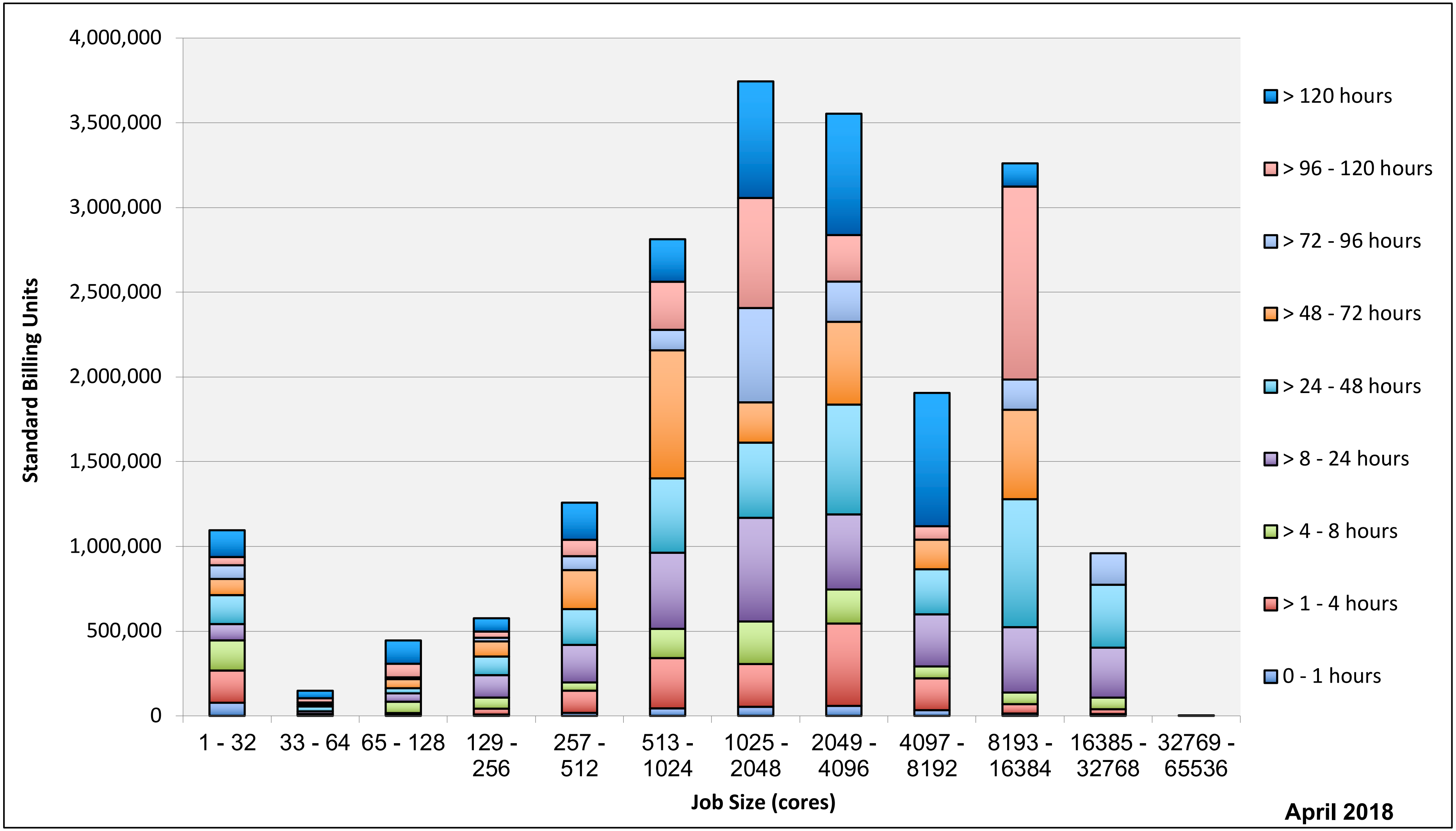
Pleiades:
Monthly Utilization by Job Length



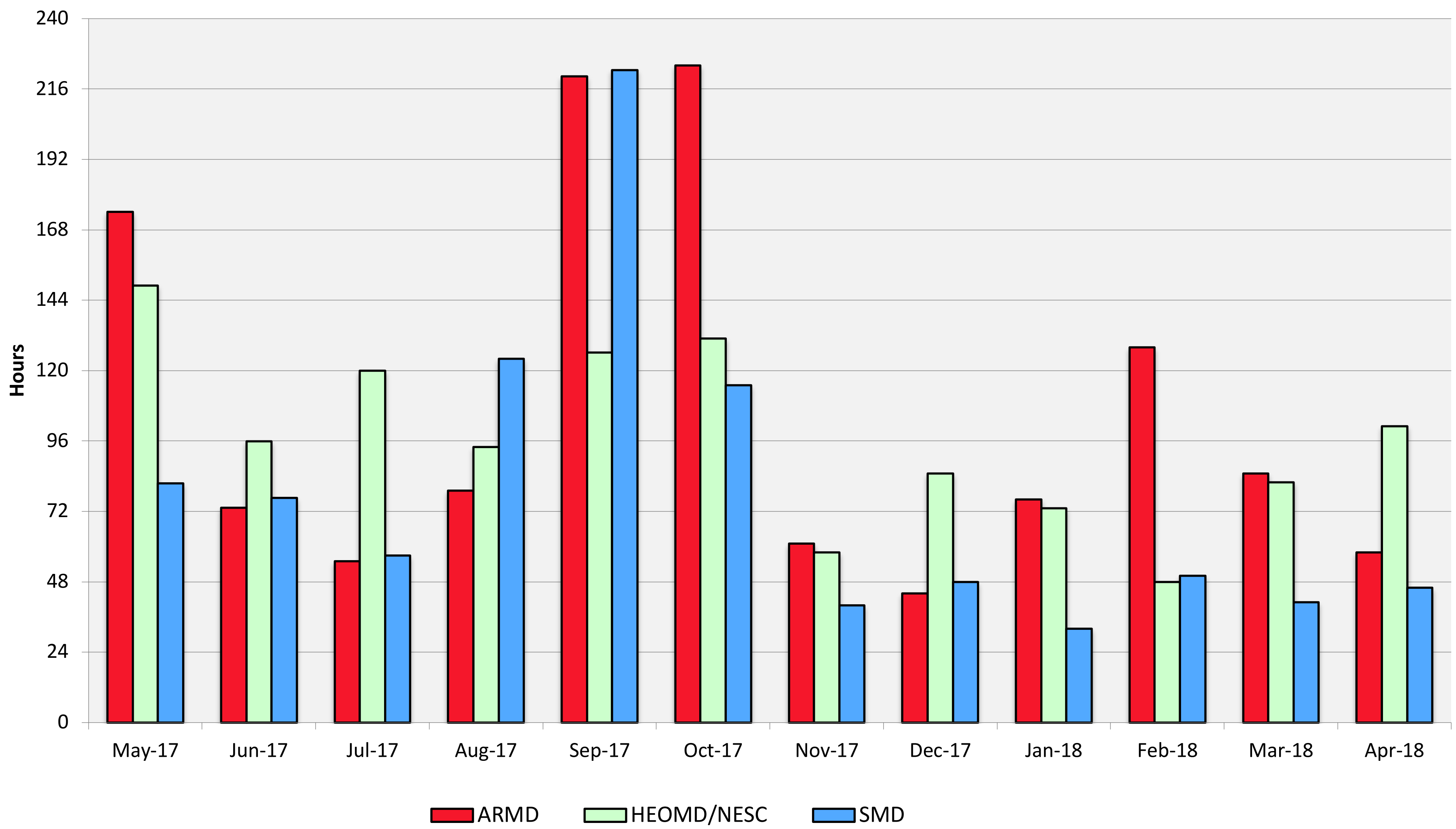
Pleiades: Monthly Utilization by Size and Mission



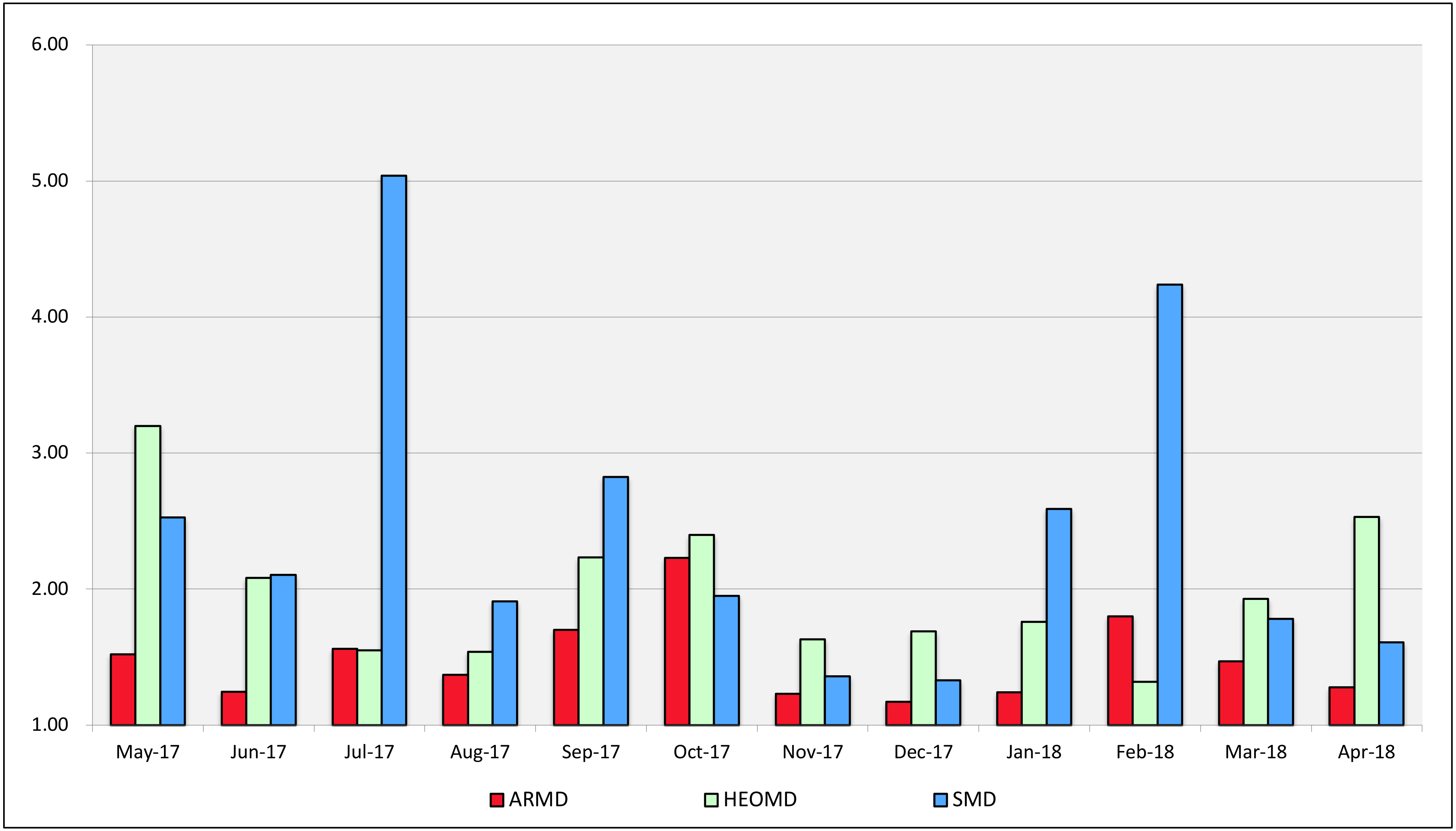
Pleiades: Monthly Utilization by Size and Length



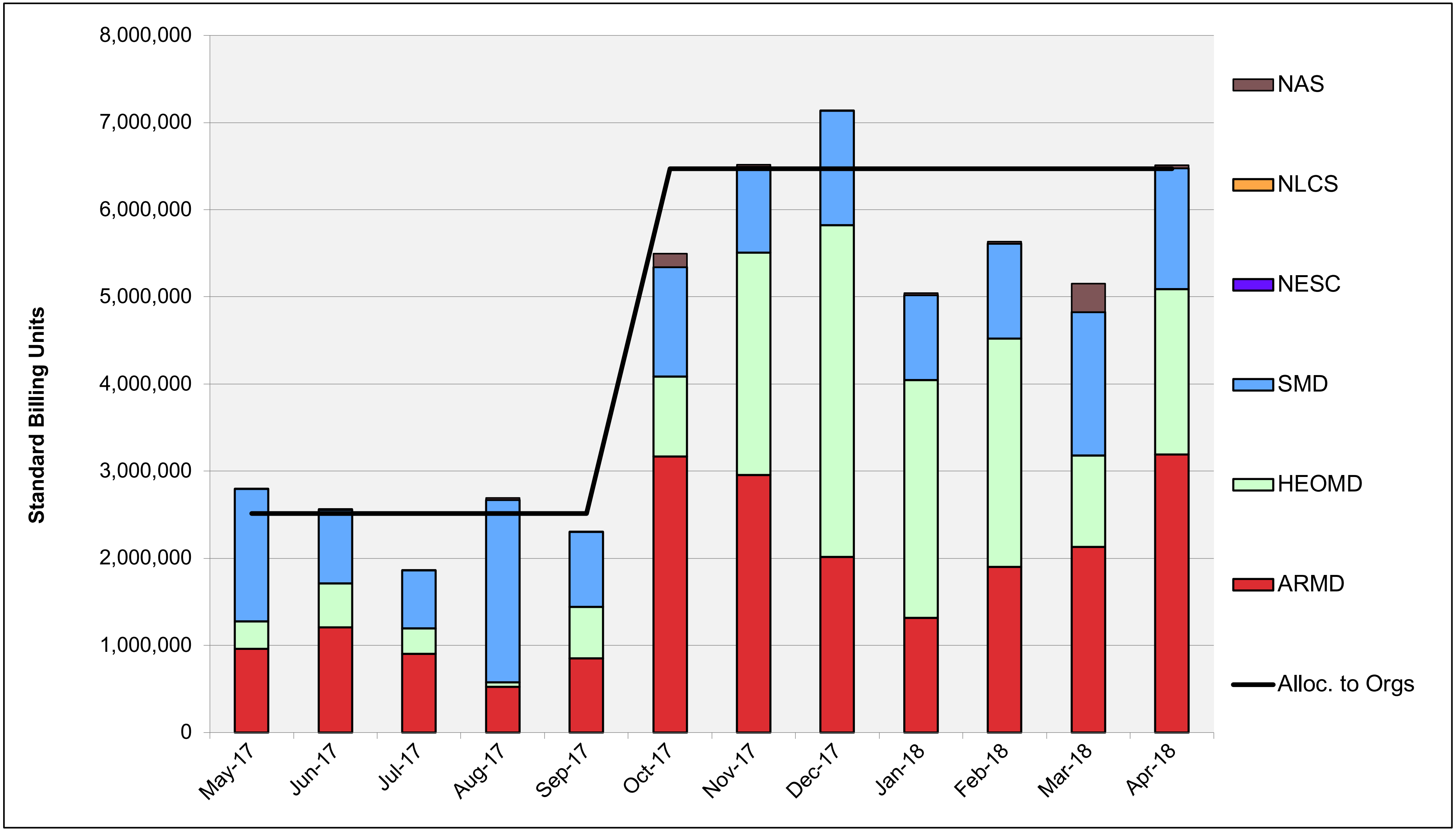
Pleiades: Average Time to Clear All Jobs



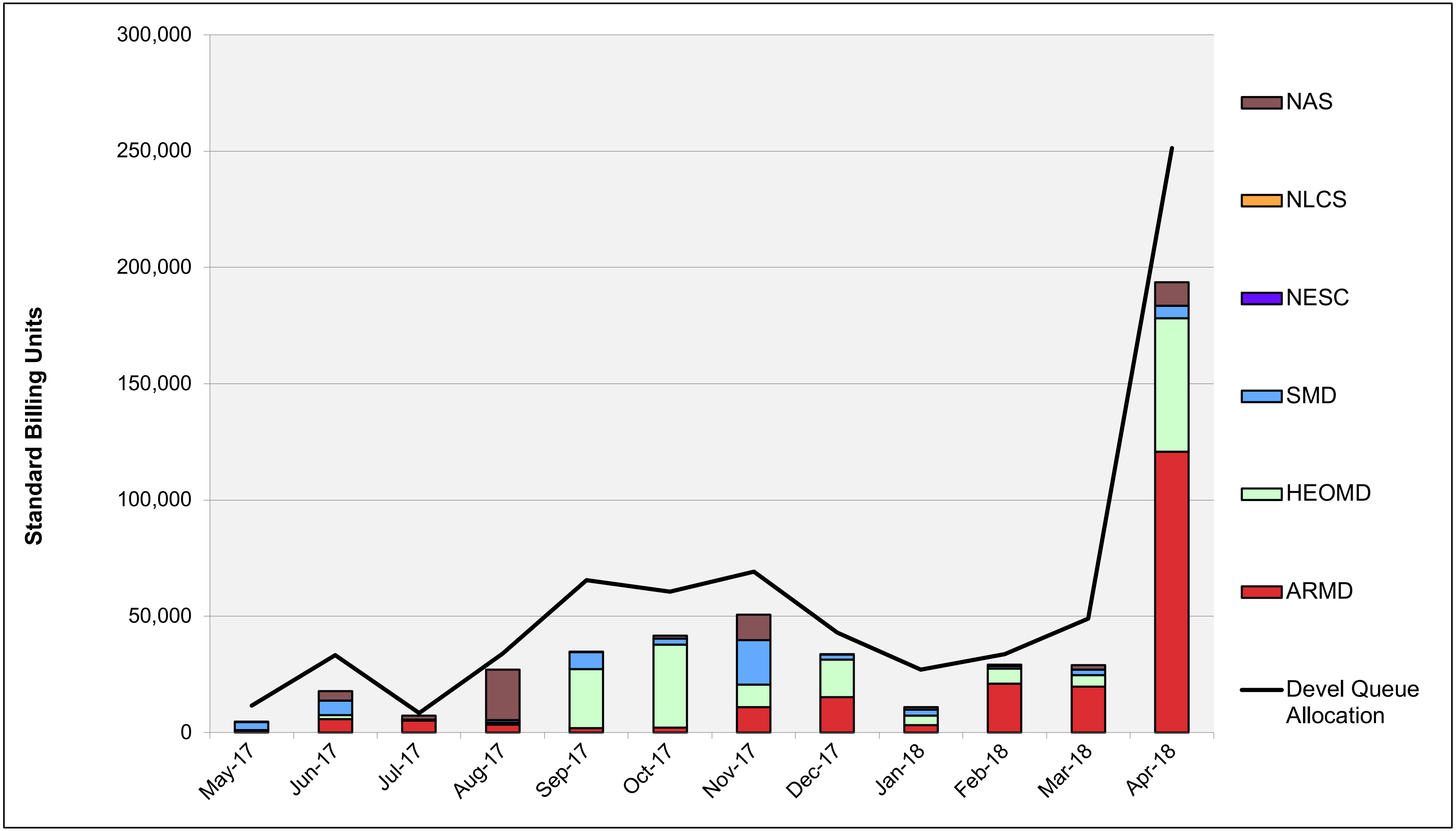
Pleiades: Average Expansion Factor



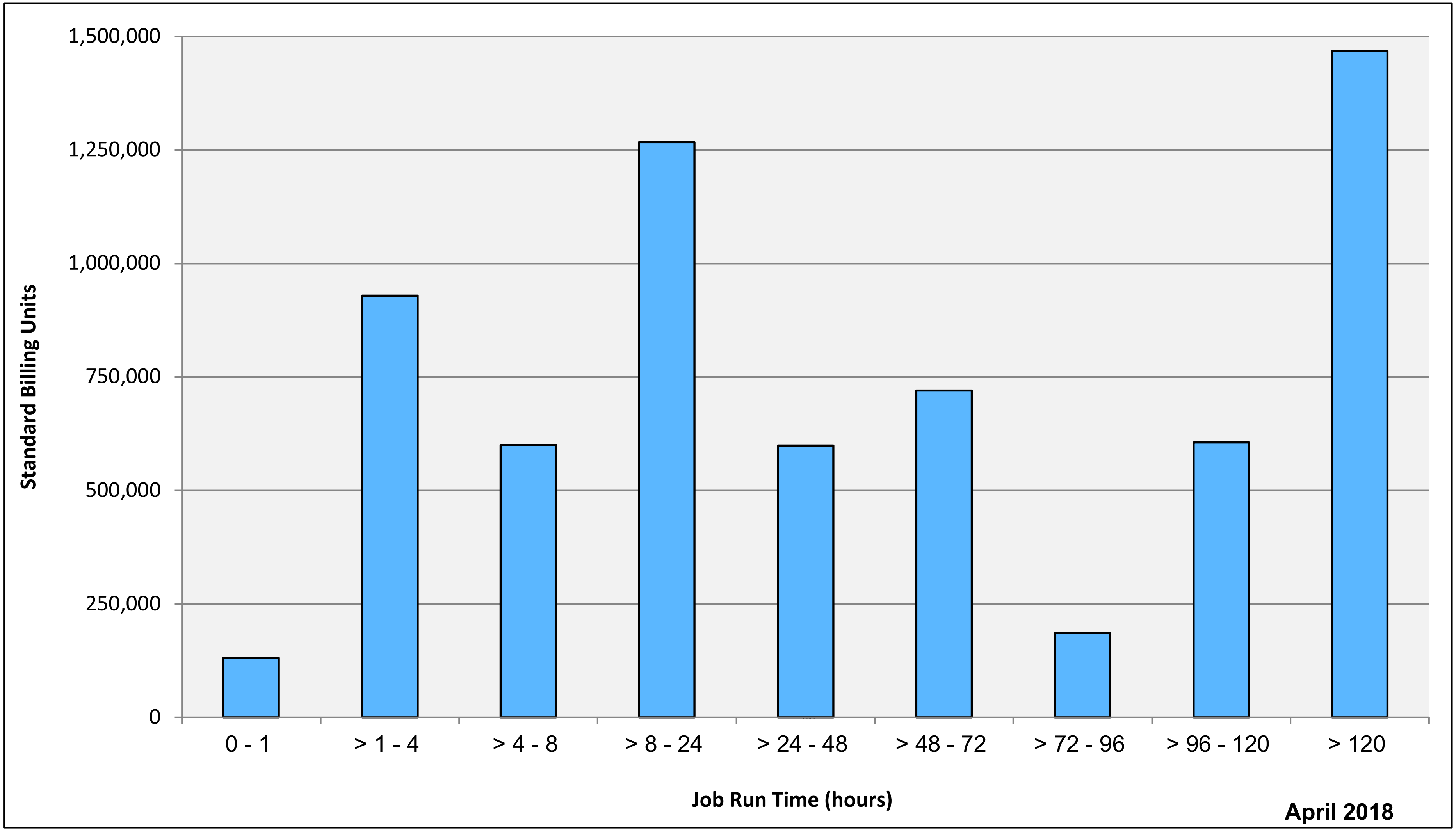
Electra:
SBUs Reported, Normalized to 30-Day Month



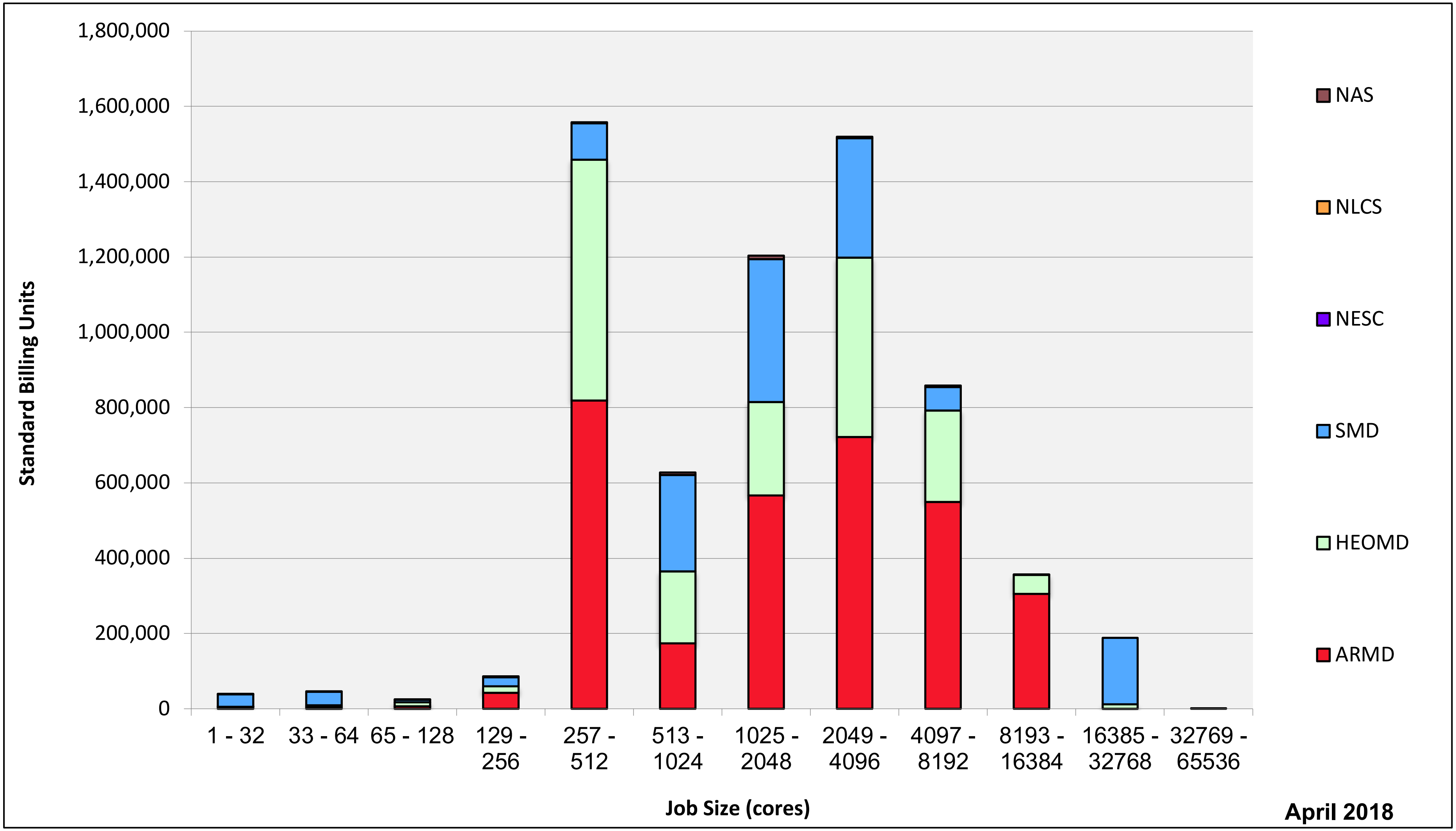
Electra: Devel Queue Utilization



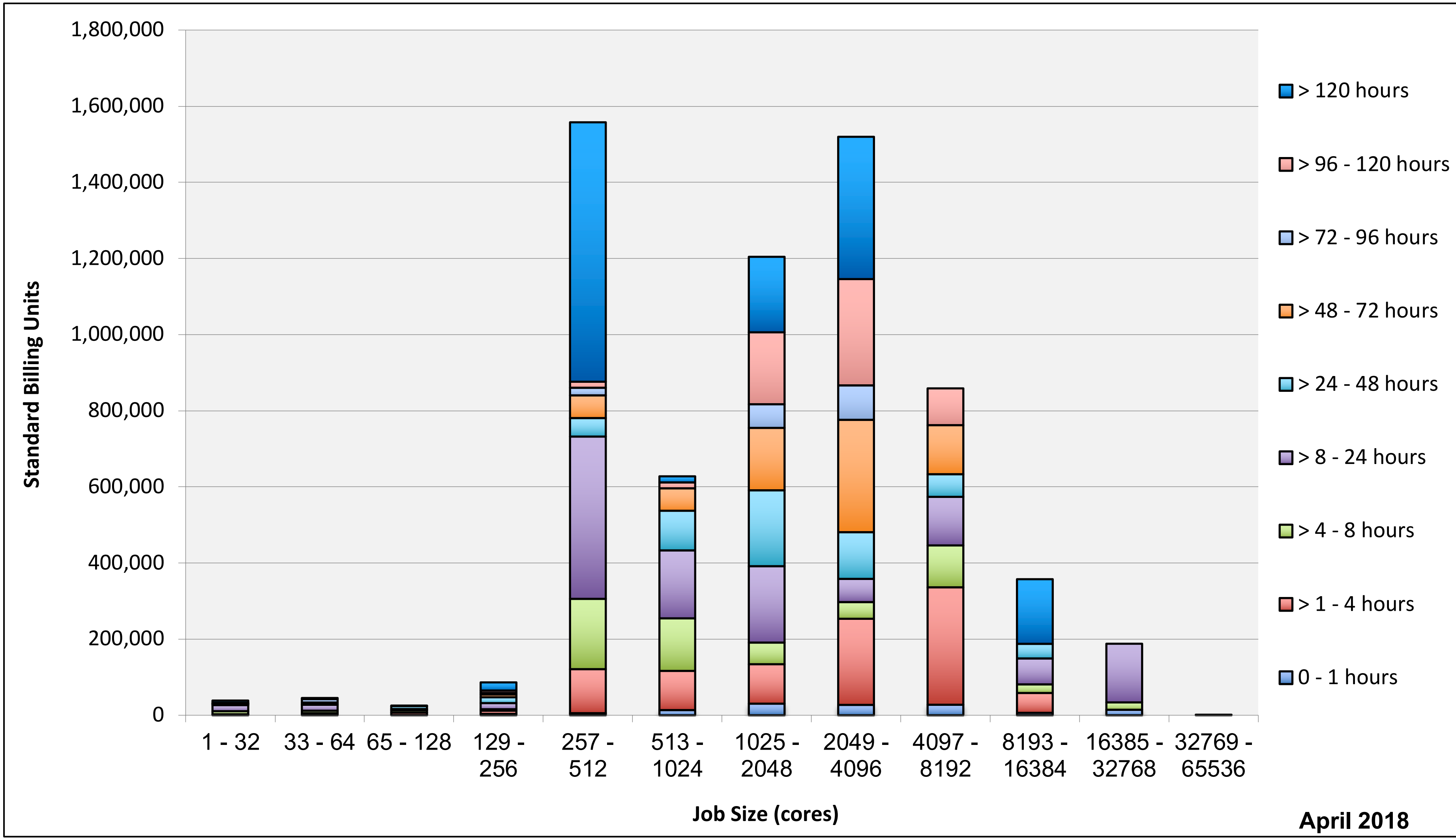
Electra: Monthly Utilization by Job Length



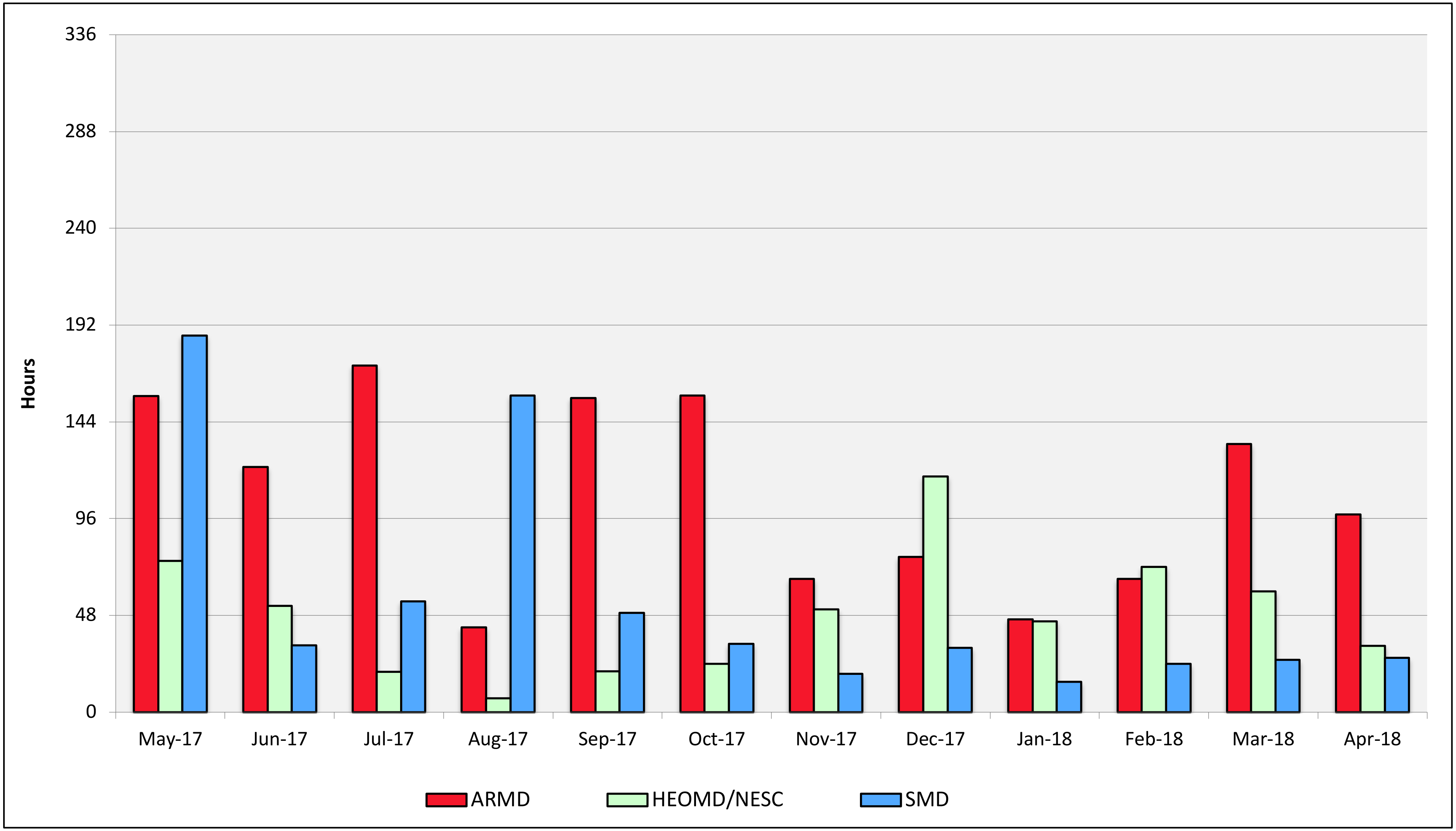
Electra:
Monthly Utilization by Size and Mission



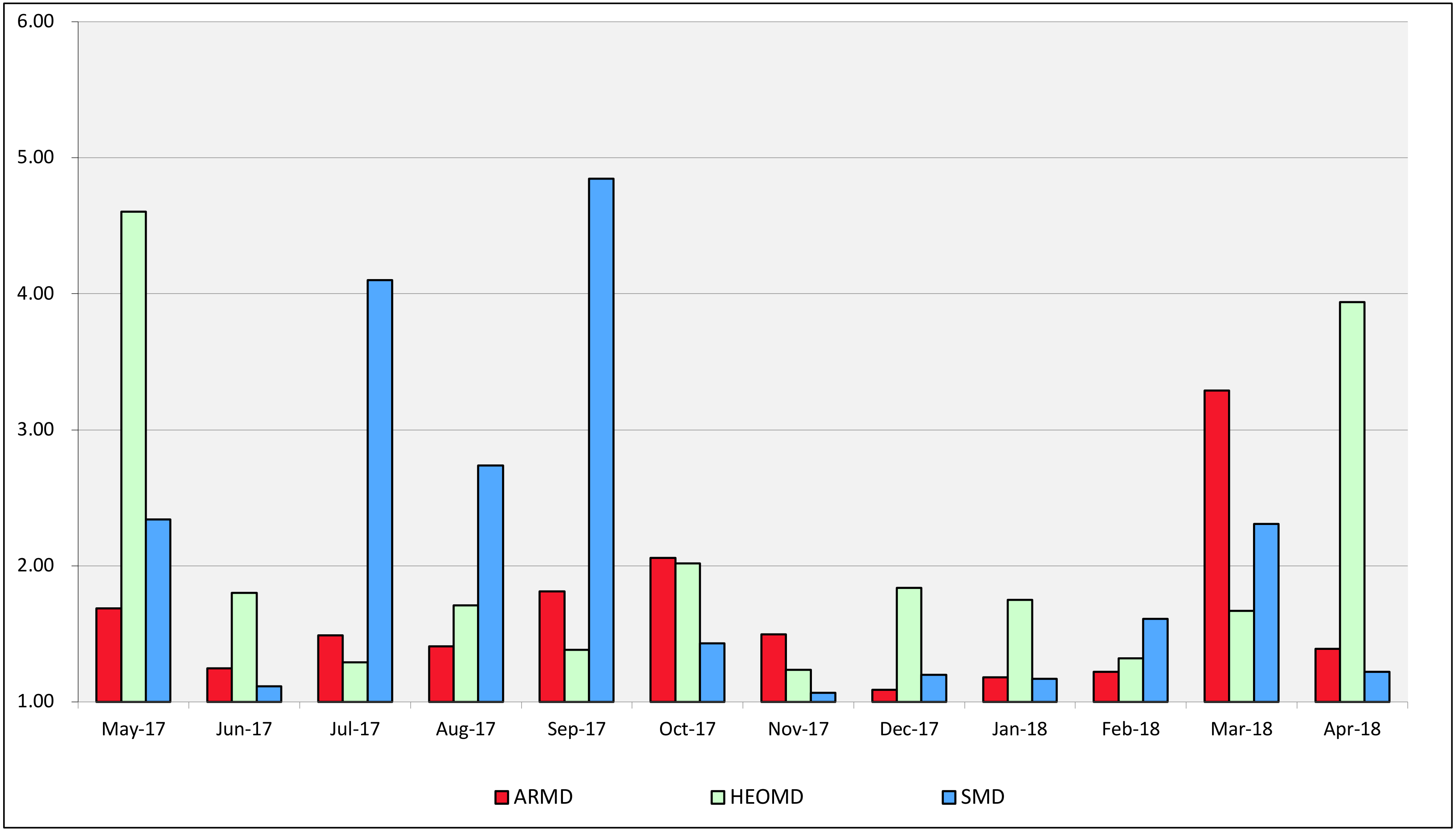
Electra: Monthly Utilization by Size and Length



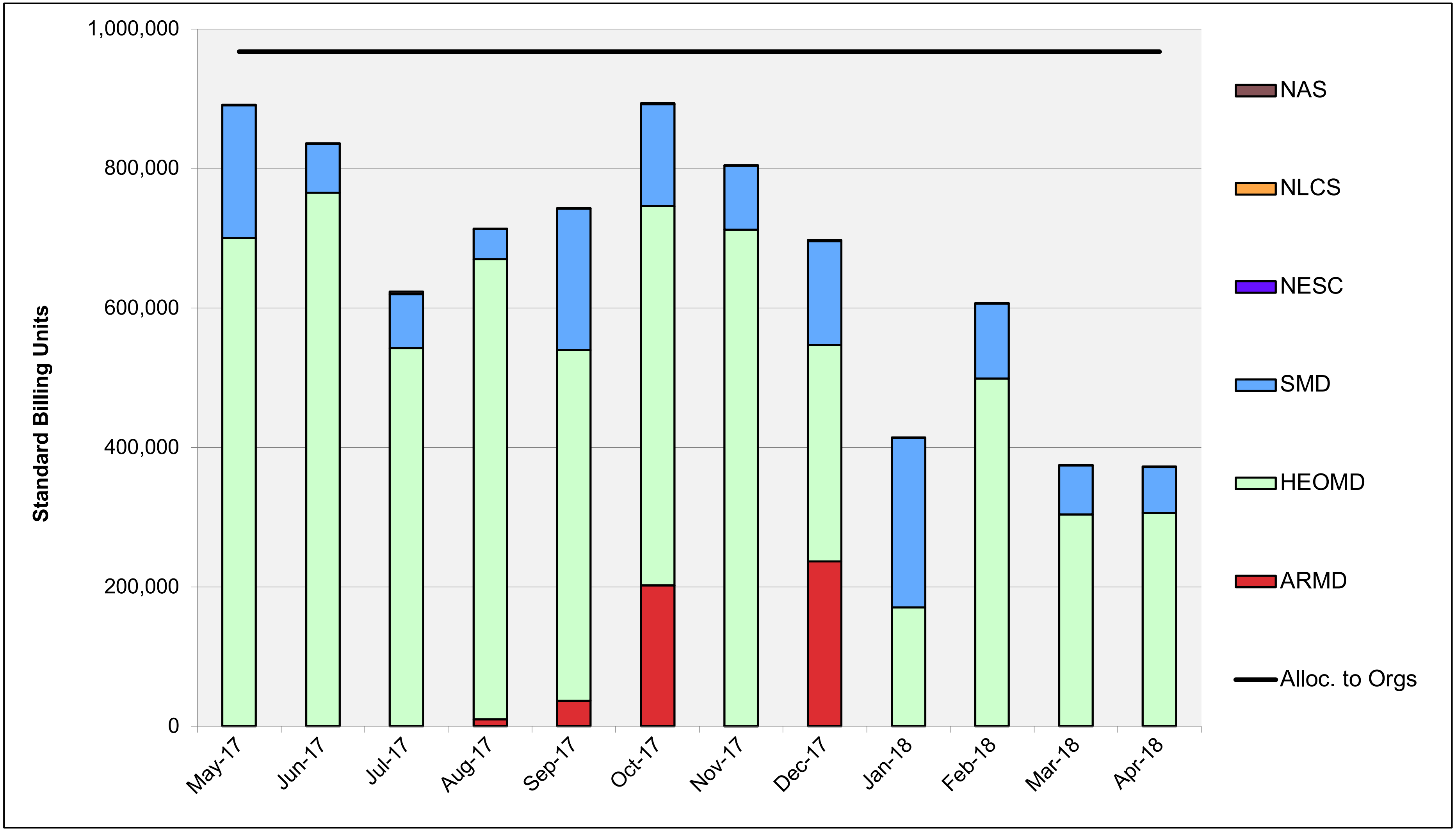
Electra:
Average Time to Clear All Jobs



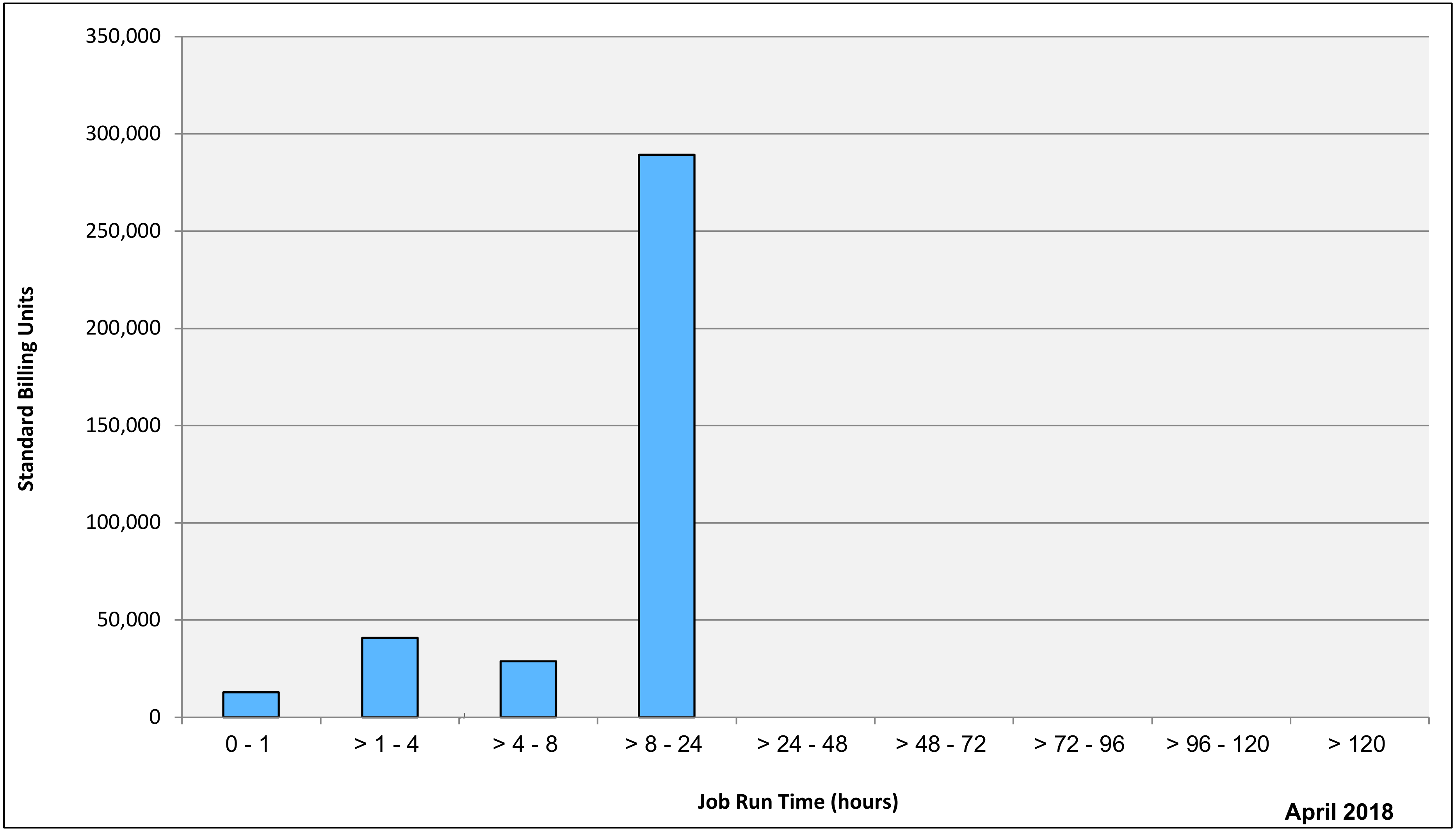
Electra: Average Expansion Factor



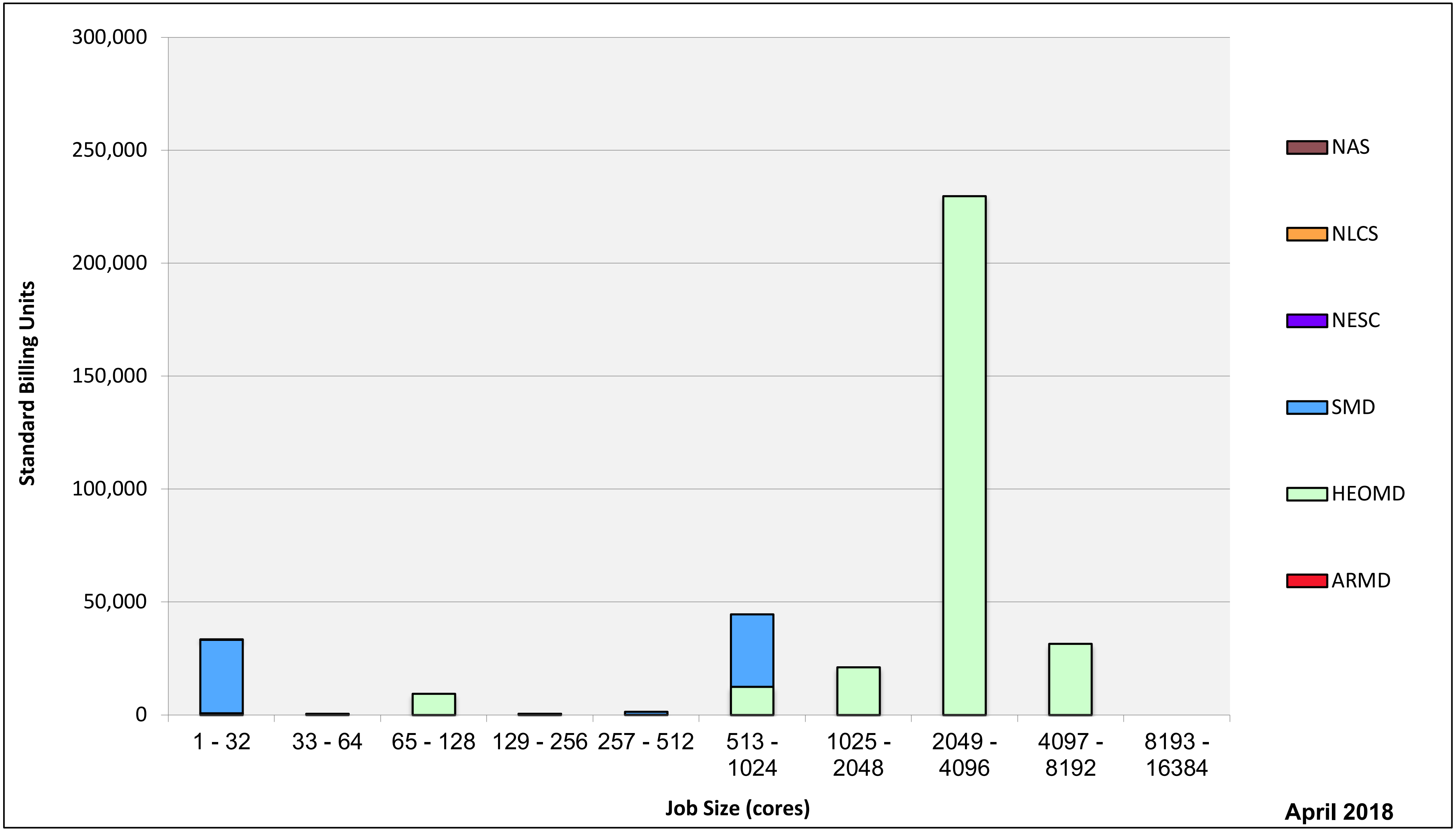
Merope: SBUs Reported, Normalized to 30-Day Month



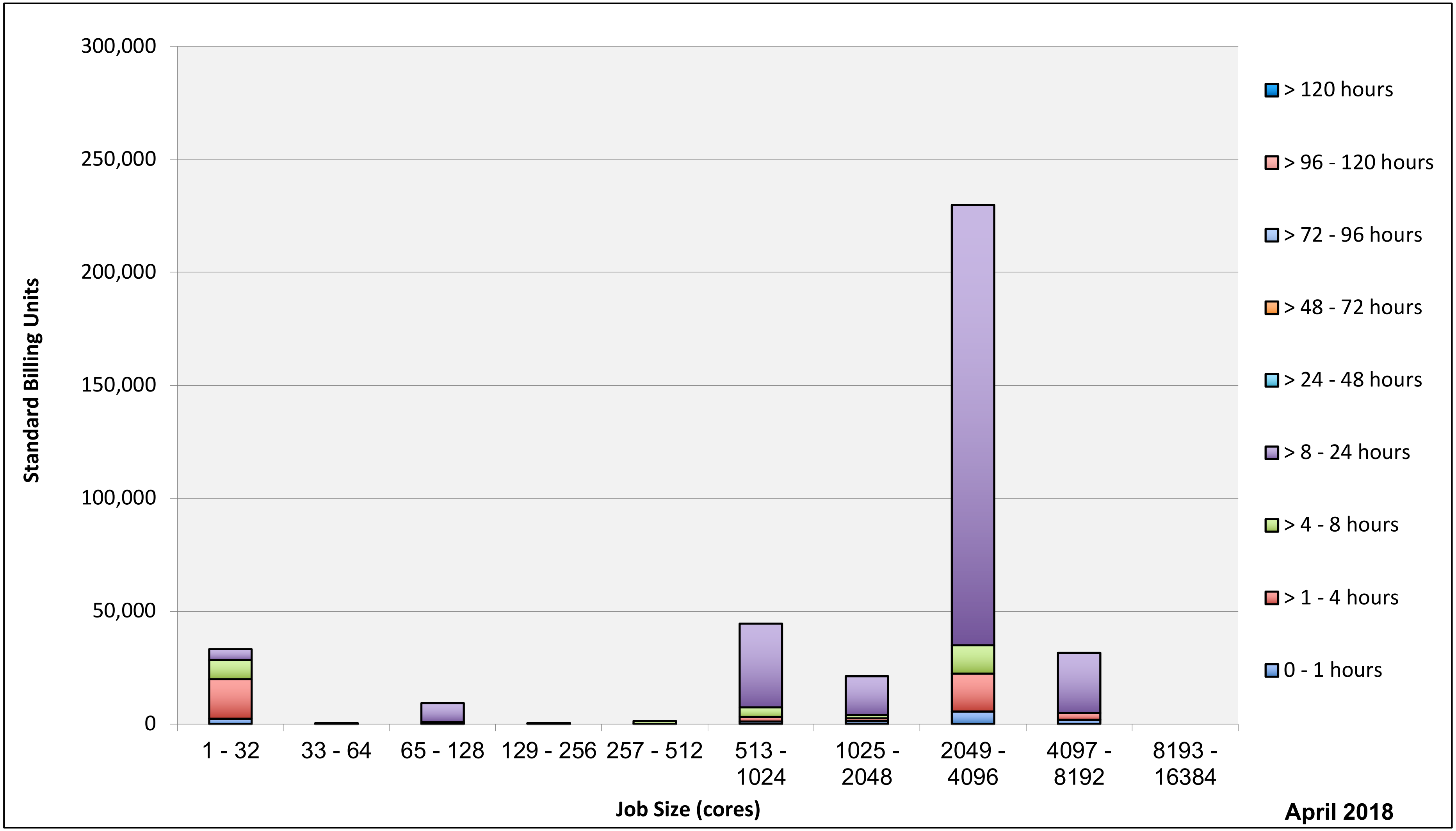
Merope: Monthly Utilization by Job Length



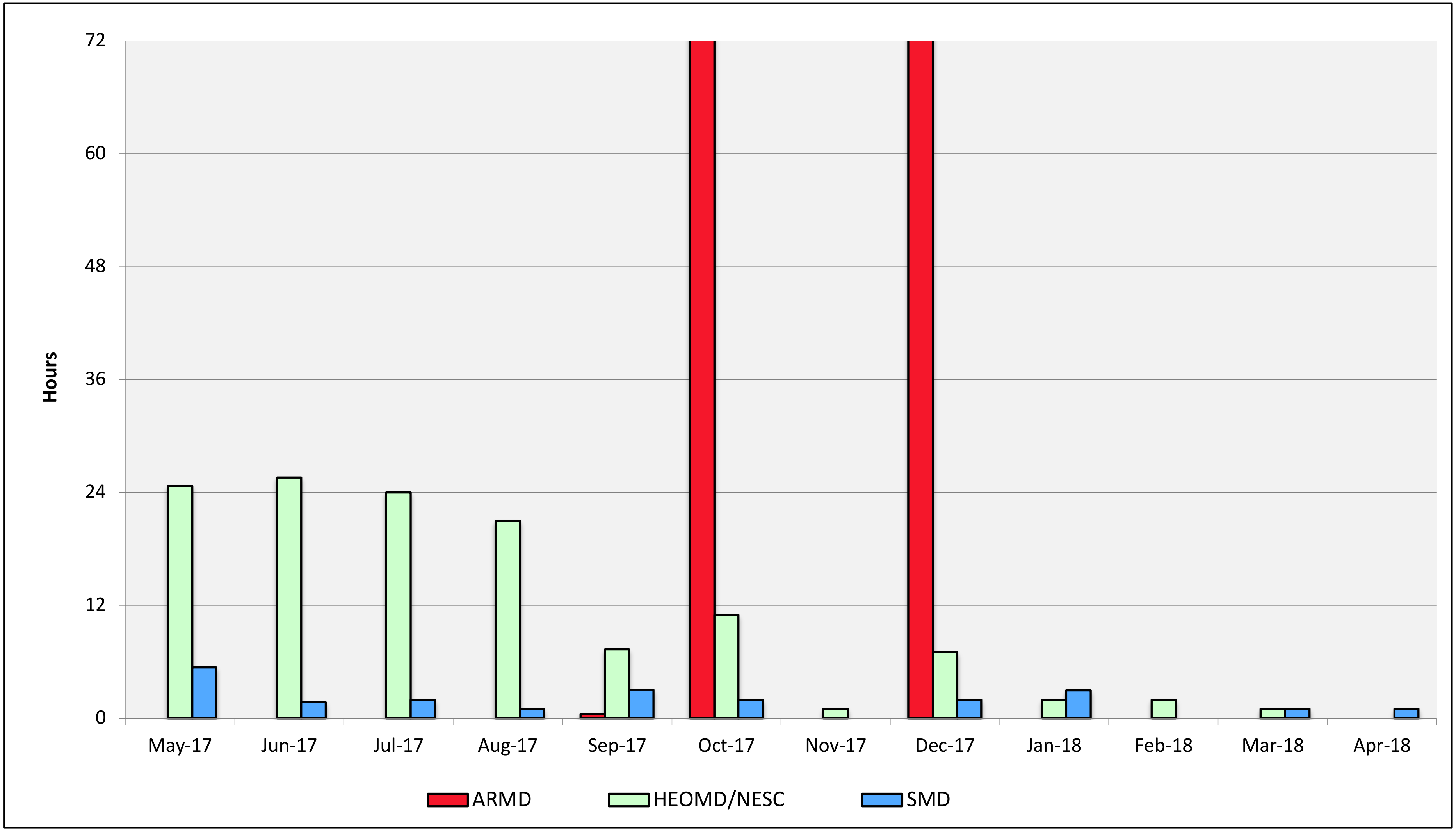
Merope: Monthly Utilization by Size and Mission



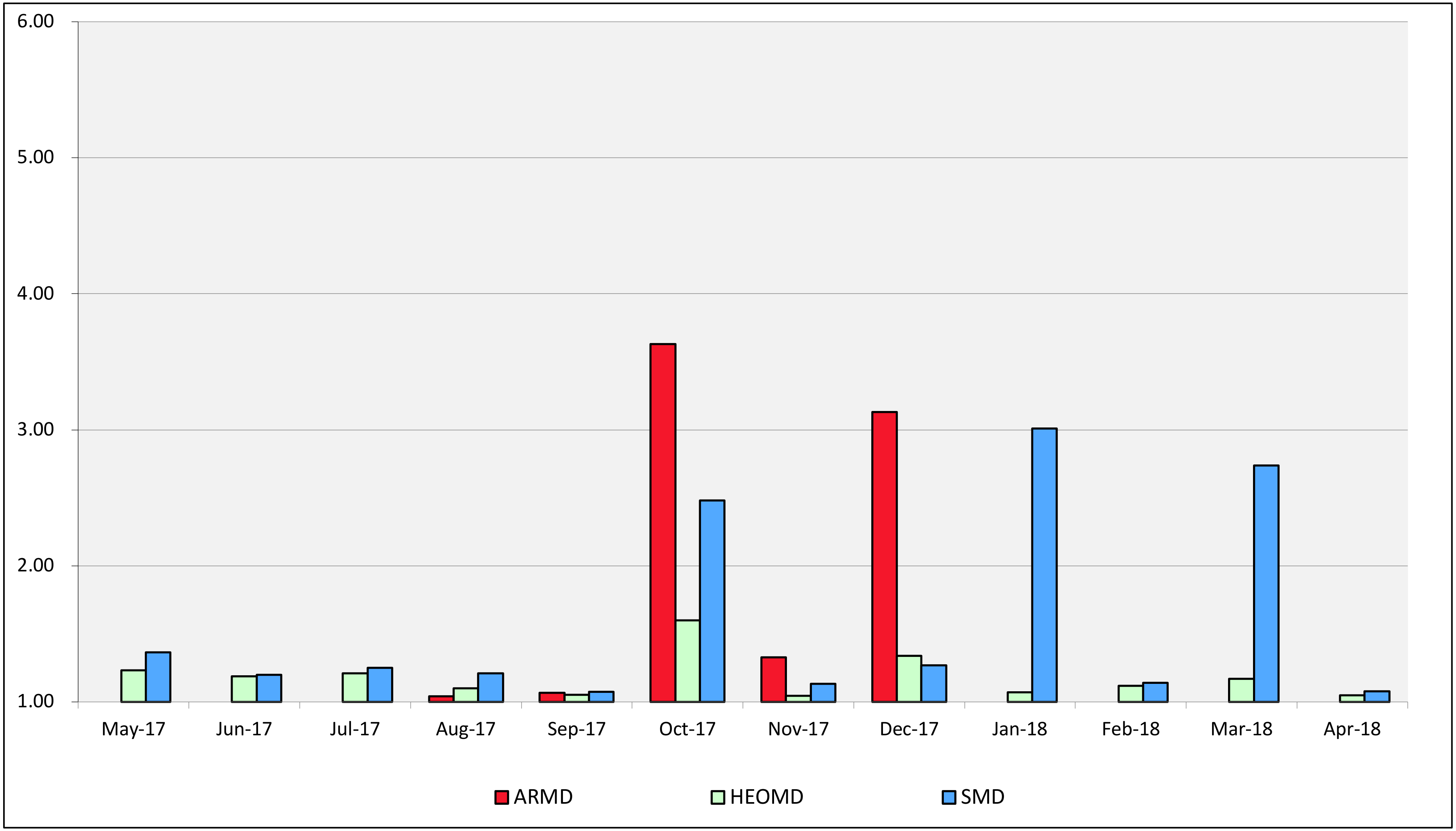
Merope:
Monthly Utilization by Size and Length



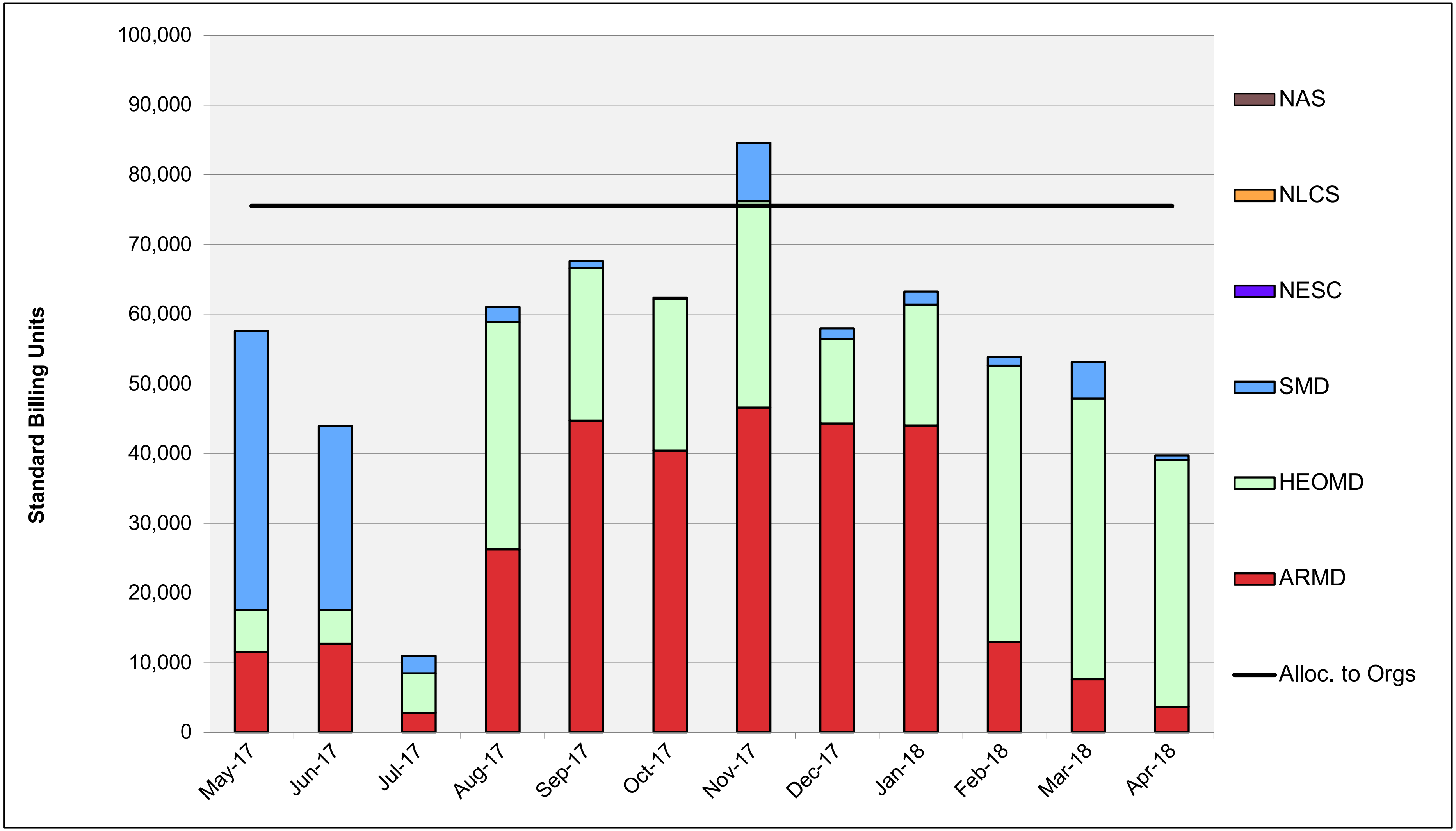
Merope:
Average Time to Clear All Jobs



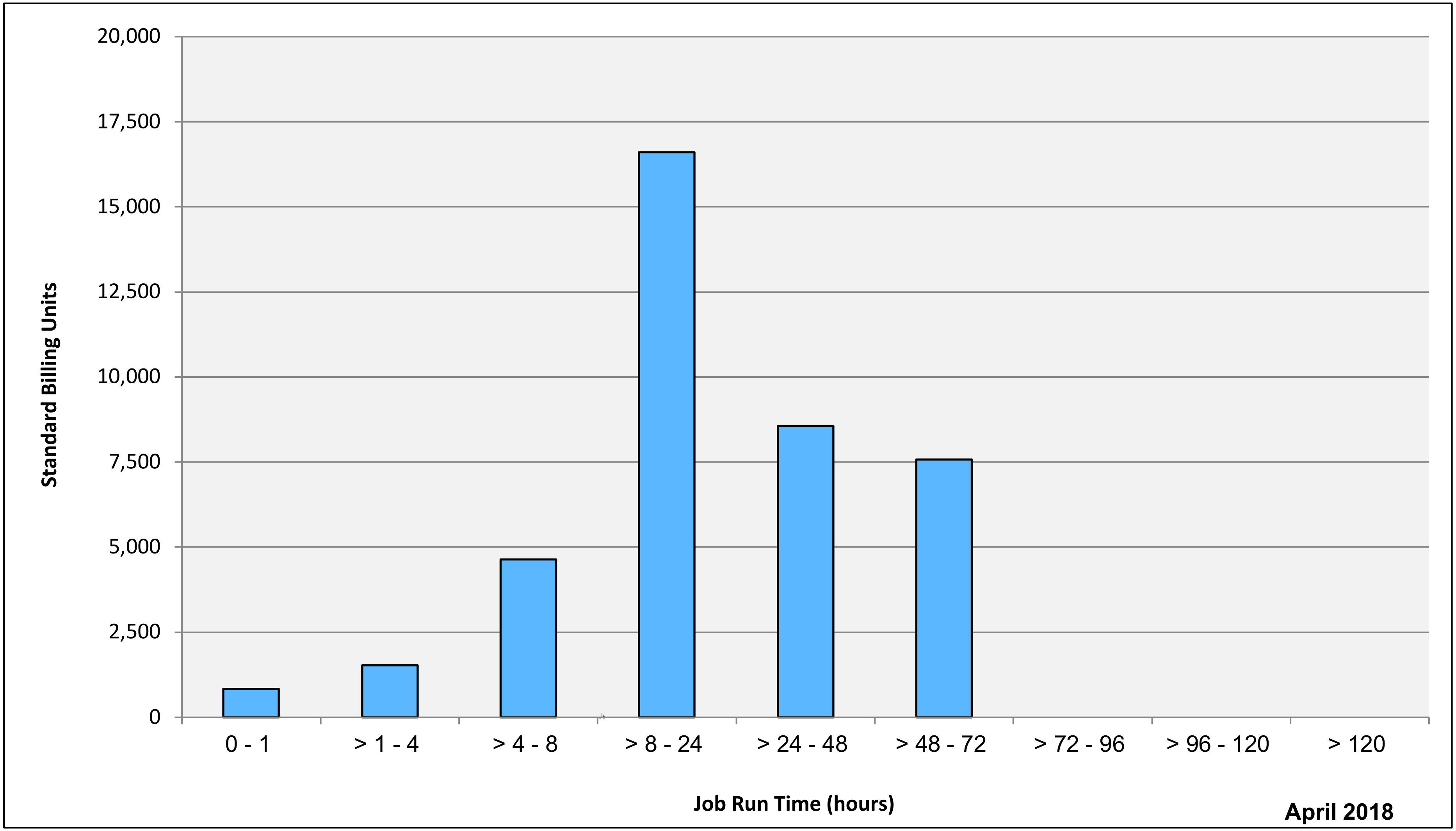
Merope:
Average Expansion Factor



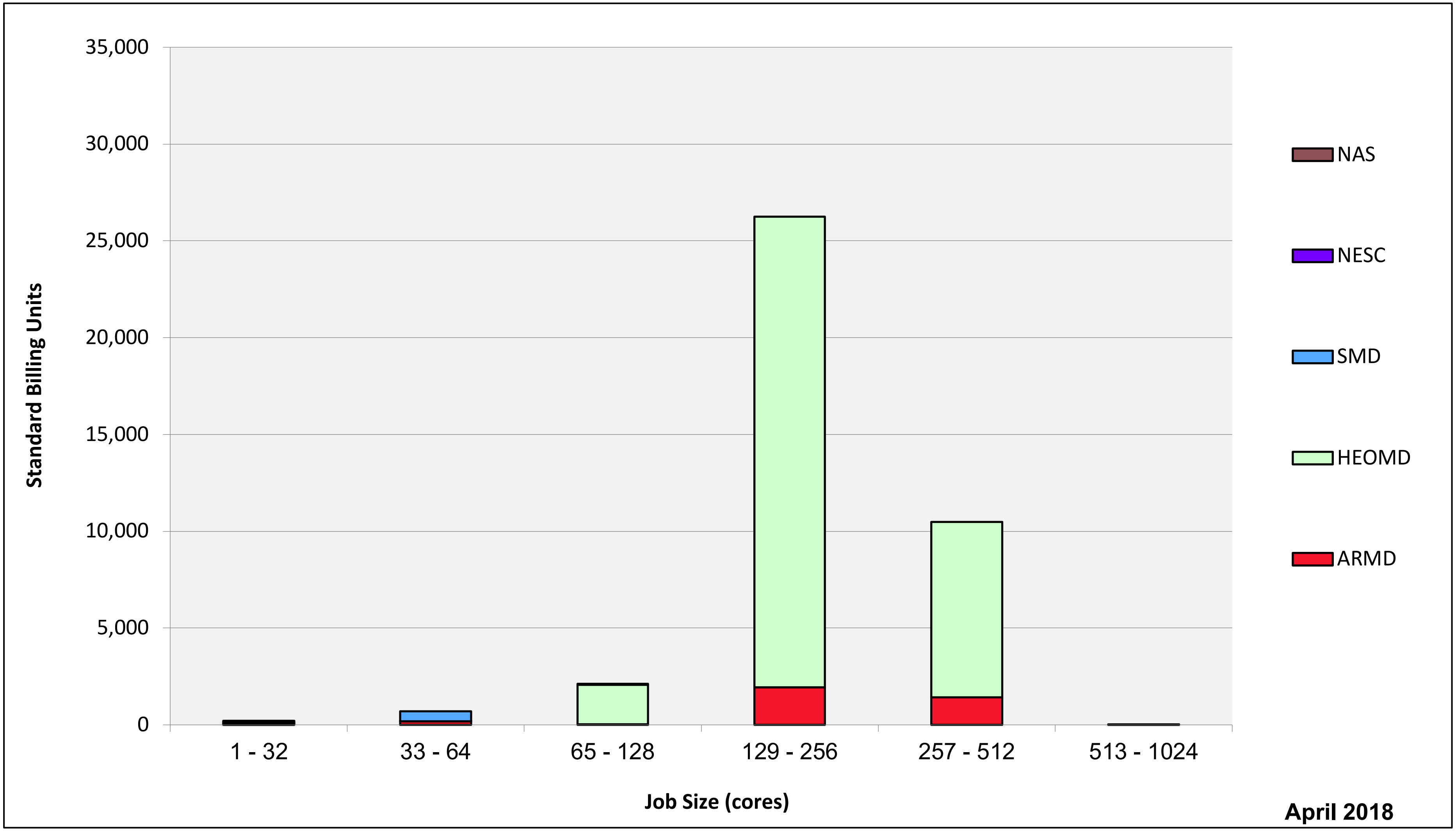
Endeavour:
SBUs Reported, Normalized to 30-Day Month



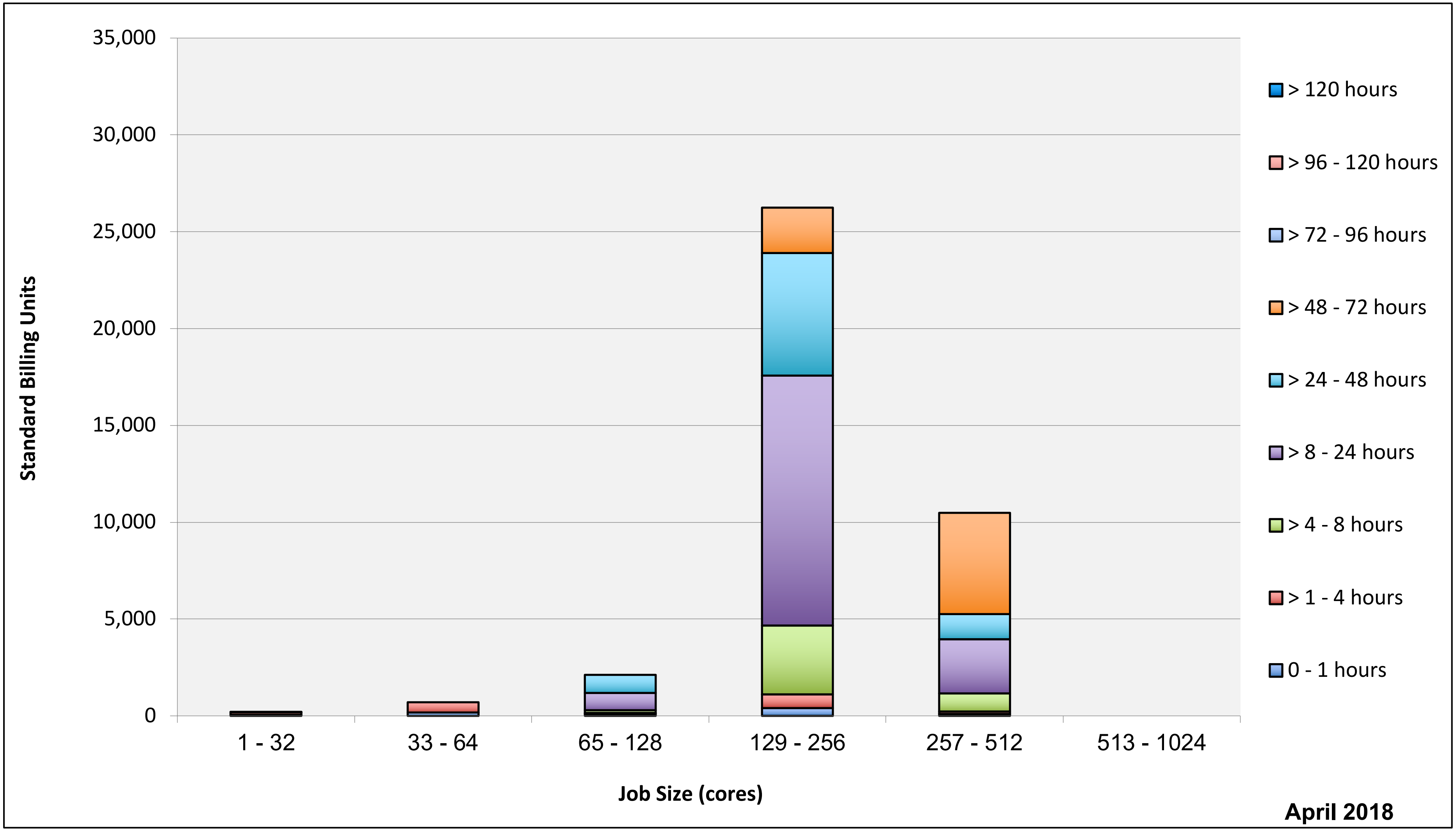
Endeavour:
Monthly Utilization by Job Length



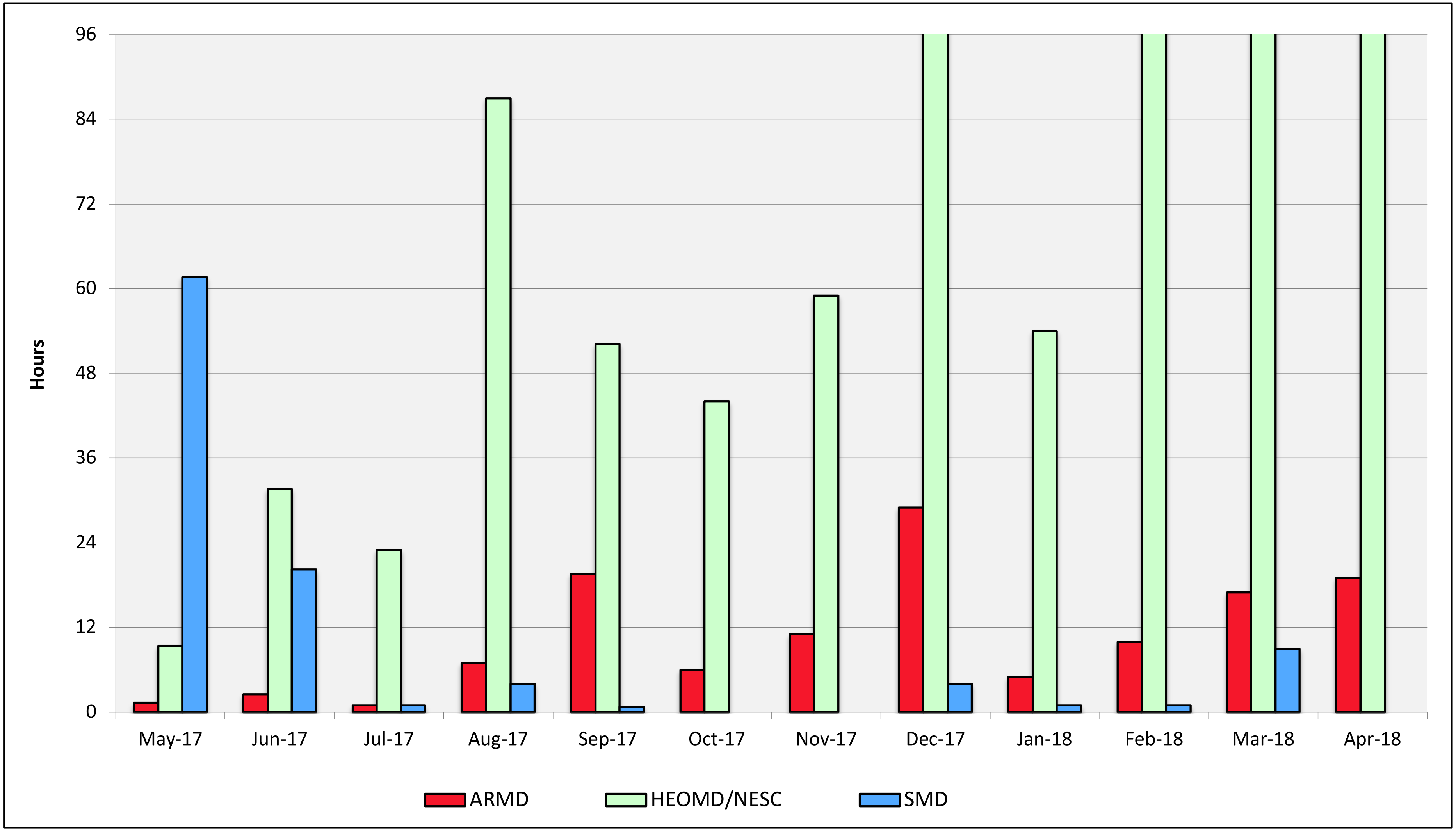
Endeavour: Monthly Utilization by Size and Mission



Endeavour: Monthly Utilization by Size and Length



Endeavour: Average Time to Clear All Jobs



Endeavour:
Average Expansion Factor