



Project Status Report

High End Computing Capability Strategic Capabilities Assets Program

August 10, 2018

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Progress Report: NAS Facility Expansion (NFE) Project



- A team of facilities, construction, and systems engineers from the HECC project, NASA Ames Facilities Engineering & Real Property Management Division, Jacobs, Tri-Technic, HPE, and Schneider Electric continued working toward completing the NFE by the end of CY2018.
- Recent accomplishments:
 - Completed the site pad: engineered fill/compaction.
 - Completed communications duct bank between NFE site and Building N258.
 - Completed electrical power duct bank on Allen Road.
 - Completed concrete foundations in Building N225B substation for transformer and dead-end structure.
 - Received & placed 30MW, 115kV – 25kV transformer, and 115kV circuit breaker.
- Near-term work:
 - Install steel “dead end” structure to support incoming 115-kV power lines.
 - Begin construction on concrete foundation, on receiving permit approval.
 - Install switchgear and 25kV power conductors in October 2018.
 - Energize the 30MW transformer and provide power to site in November 2018.

Mission Impact: The NAS Facility Expansion project will enable HECC to vastly increase its computational and storage capacity, enabling users to produce even more world-class science and engineering results for NASA missions.



A 30-megawatt transformer is lifted off the delivery truck via crane and placed on the concrete transformer foundation at the N225B Substation site, on July 16, 2018.

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Electrical Power Protection Fully Restored in Main Supercomputing Facility



- The HECC Facilities team, in collaboration with technicians from NASA Ames Facilities Engineering & Real Property Management Division, Jacobs, and Hitec, completed repairs on the Rotary Uninterruptible Power Supply (RUPS) for Building N258 and returned all three units to full operation.
- RUPS #1 was repaired with a new induction coupling and rebuilt generator; five-year maintenance was completed on the diesel engine.
- RUPS #2 & #3 induction coupling bearings were re-greased to maintain their smooth rotation, and the annual maintenance service was completed to reduce the risk of failure.
- The N258 building load of 5.5MW is now completely protected by the 6MW RUPS.
- In addition to uninterruptible power, the RUPS conditions the incoming power to N258, protecting against spikes and dips and improving HECC's compute availability.

Mission Impact: Protecting HECC resources in NASA's largest supercomputing facility provides reduced risk of failure due to power outage events, and increases resource availability for NASA users.



The interior of RUPS unit #1. Gray hardware in the foreground (right) is the diesel engine; blue hardware in the middle is the induction coupling; and blue hardware in the background is the generator. Each RUPS unit has a 20-megawatt capacity.

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New Lustre Filesystem Deployed for NASA Earth Exchange Users



- The HECC Supercomputing Systems team deployed the first in a series of seven additional Lustre filesystems for users.
- This first filesystem is dedicated to the NASA Earth Exchange (NEX) project, which provided funding for the filesystem.
- The remaining six filesystems will be accessible to the general user community.
- The total storage capacity procured was 23 petabytes (unformatted), with an expected usable 16 petabytes.
 - The storage will be split between the seven filesystems, with a capacity of up to 4.8 PB and 14 gigabytes per second of bandwidth.
- The remaining filesystems will be rolled out in stages. When all are deployed, two of the oldest Lustre filesystems will be retired and the user data migrated.
- The data migration will be completed as transparently as possible to minimize the impact on user workflow.

Mission Impact: The new filesystems will help keep up with users' demand for a larger, high-performance storage capability to run more data-intensive applications, and enables researchers to make the best use of HECC supercomputing resources.



The HECC Lustre filesystems consist of 10 RAID units, each with 230 disk drives and 20 servers.

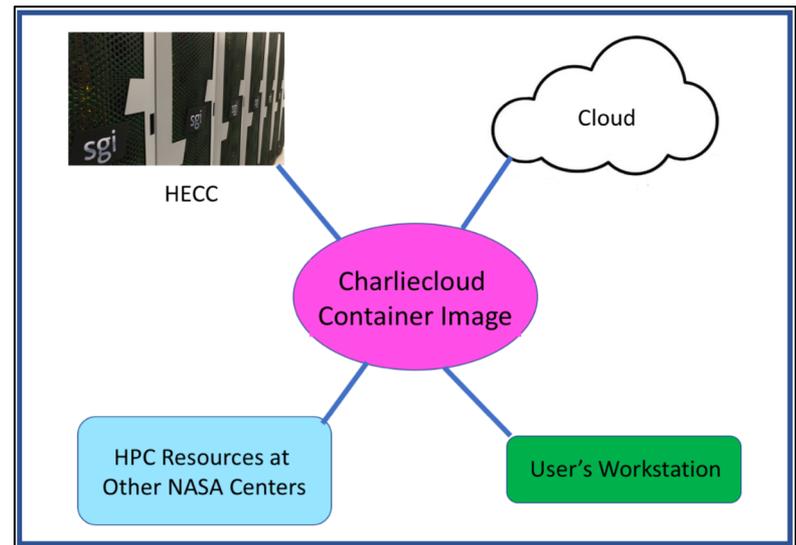
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User-Defined Software Stacks Enabled Through Charliecloud Containers



- HECC engineers evaluated and deployed Charliecloud, a light-weight container technology, for users who want to bring their own software stacks for validity, portability, and consistency.
- Charliecloud, developed by researchers at Los Alamos National Laboratory, is built on top of Docker, a commonly used open platform to build, ship, and run distributed applications.
- The Supercomputing Systems team provided two methods to create a Charliecloud container image:
 - Build on Pleiades without root privilege through an HECC-supplied CentOS 7 operating system base image.
 - Build on the user's root-privileged private workstation with a Dockerfile.
- The Application Performance and Productivity (APP) team successfully validated the two methods with multiple applications, such as Intel Distribution for Python and OpenFOAM MPI (single node only), on both Pleiades and the Amazon Web Services (AWS) cloud. Four HECC Knowledge Base articles were created and published in mid-July.

Mission Impact: Enabling user-defined software stacks allows users full control of their environments, and reduces the workload of HECC staff to create and maintain numerous complex software environments for different users—freeing time to provide in-depth, custom support to users.



A Charliecloud container image is self-contained and portable across multiple platforms, relieving researchers from the need to rebuild and/or revalidate each of them.

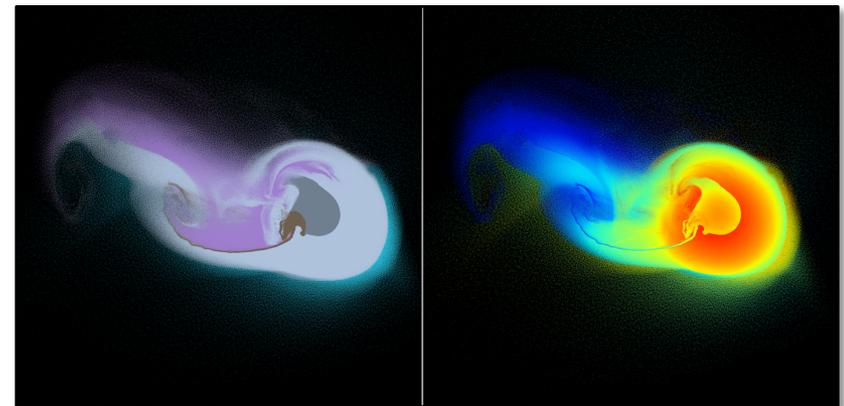
POCs: Jeffrey Becker, jeffrey.c.becker@nasa.gov, (650) 604-4645, NASA Advanced Supercomputing (NAS) Division;
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Applications Experts Advance Giant Planetary Impact Simulations with Electra Skylake Nodes



- HECC Application Performance and Productivity (APP) experts provided in-depth support for researchers from Durham University, UK and the Bay Area Environmental Research Institute/NASA Ames to port, optimize, and scale the SWIFT cosmology simulation code to Pleiades and Electra.
- The researchers' high-resolution simulations of giant impacts on Uranus use 10 –100 million particles and originally took 8.9 seconds/time step. APP assistance included:
 - Switching to the Intel compiler and hyperthreading (48 threads), which improved this to 6.6 secs/step.
 - Turning on extra compiler flags further improved this to 5.3 secs/step.
 - Switching to running hyperthreaded on a single Skylake node attained 2.7 secs/step.
- APP determined that the Skylake nodes, with their large number of cores (40) per node accessing localized memory, are ideal for these particular simulations: the high core count enabled testing of many impact scenarios with minimal communication costs— one job per node.
 - Most of the particles are in a tiny section of the simulation box, so most of the simulation volume is empty space.
 - SWIFT's MPI parallelization involves spatial cuts, so particles interacting with their neighbors are all on one chip, to minimize communication costs.
- Bottom line: scaling with threads is much better than with MPI ranks due to the difficulty in distributing the workload between ranks.

Mission Impact: HECC's faster, high-core-count Skylake nodes are ideally suited for this kind of research requiring testing many different impact scenarios in an “embarrassingly parallel” way with minimal communication costs.



Unlike other planets in the solar system, Uranus spins almost on its side. Scientists believe that a young proto-planet of rock and ice collided with Uranus four billion years ago, causing its extreme tilt. This image shows a mid-collision on Uranus. The left-hand panel is colored by material (light/dark gray represent ice/rock on Uranus, purple/brown represent ice/rock from the impactor, light blue represents Uranus' atmosphere). The right-hand panel shows internal energy distribution.

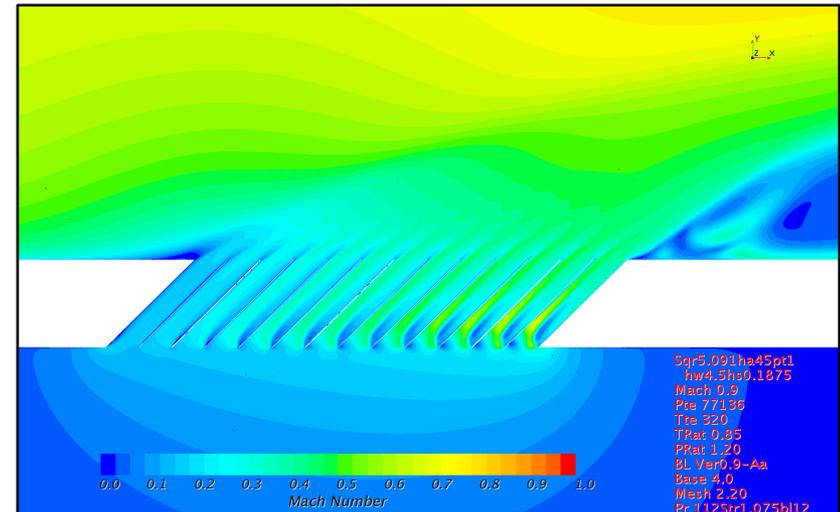
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APP Team Finds Elegant Solution to Enable STAR-CCM+ to Run on Electra Skylake



- For months, NASA Ames aerospace engineer Michael Schuh tried to run simulations for a Space Launch System rocket venting design on Electra Skylake nodes using STAR-CCM+, a commercial-off-the-shelf CFD code, but frequently encountered MPI initialization failures. The code runs fine on all other node types, but Code AA funded 34 new Skylake nodes for Electra, so solving the problem became urgent.
- Once the HECC APP team got involved, they worked with Schuh to find a solution.
 - Determined the root cause of the job failures was due to a mix of nodes from the Skylake “A” and “B” blades. Only the Skylake nodes (in E-cells) have this A/B double-density configuration, with different subnet prefixes for ib0. This confused the Platform MPI library in STAR-CCM+.
 - Tried to modify the STAR-CCM+ scripts and insert HPE’s perfboost tool to translate all MPI calls into HPE’s MPI calls, which can handle mixed subnet prefixes. This proved infeasible due to the complicated scripts—starccm+ and setup parallel scripts account for a total of 4,230 out of more than 16,000 lines of scripting logic.
- APP experts and Schuh found the solution while scrutinizing the scripts.
 - Discovered that STAR-CCM+ also supports SGI MPT, and identified the appropriate environmental settings and command line options.
 - Created a private HPE MPT module for Schuh and colleagues, necessitated by STAR-CCM+’s hard-coded MPI launcher, which differs from that in the HPE/SGI MPT modules.

Mission Impact: HECC applications experts work closely with users to find custom solutions to running important codes for NASA space exploration missions; and, in this case, save users’ time by making it much easier to maintain future releases of commercial-off-the-shelf software.



Flow through a novel, 13-channel honeycomb vent to improve venting of interstitial air for the Space Launch System rocket. Colors show flow Mach number from interior region of the rocket (bottom) through the honeycomb into Mach 0.9 freestream air (above). White regions (left and right of the honeycomb vent) are the rocket shell.

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Security Team Leads Contingency Plan Exercise to Ensure Incident Preparedness



- The HECC Security team prepared for and led a tabletop exercise with representatives of every technical area at the NAS facility.
- The exercise described a scenario of a security incident and each representative described how they would respond to the incident.
- The scenario involved evidence of an Advanced Persistent Threat (APT) discovered in HECC systems and, as a result, the NAS facility was disconnected from the external networks.
- The groups worked together to determine how to resolve the issue, reduce downtime for systems and users, and reconnect back to external networks.
- The exercise was very successful, and demonstrated that HECC has a solid plan for handling contingencies when incidents arise.

Mission Impact: Successful completion of NASA's annual contingency plan test helps the HECC project maintain its authorization to operate agency supercomputing resources.



Protection of NASA's supercomputing assets is of paramount importance to all HECC support staff.

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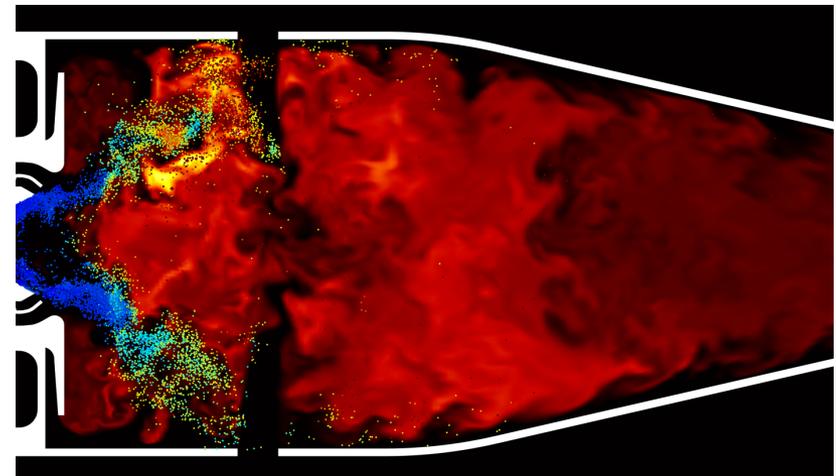
Pleiades Enables Simulation of Next-Generation Clean, Sustainable Jet Fuels*



- As part of a collaboration with NASA, the FAA, and industry partners, researchers at Stanford University developed state-of-the-art, multiphysics simulations to investigate new jet fuels and compare their performance with current fuels.
- New fuels must go through an extensive certification process, including small- and large-scale experimental validation, which is expensive and time consuming.
- The simulations, run on Pleiades, determined the relative performance of new fuels at operating conditions near lean blowout (LBO), where combustion can be highly unstable.
 - The researchers' flamelet/progress-variable combustion model accurately reproduced experimental LBO behavior of the candidate fuels; and showed how fuel evaporation rate, gaseous-fuel deposition, and flame anchoring were affected by specific fuel properties.
- This study was the first step to demonstrate that CFD tools can be used to screen candidate fuels within the certification process to reduce cost and time requirements.

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

Mission Impact: HECC supercomputing resources and data storage capability enabled researchers to run massive simulations for realistic jet engine configurations for screening new candidate jet fuels.



Snapshot of a model jet engine simulation, highlighting the temperatures (black-red/yellow) within the combustion chamber and the liquid fuel droplets (small dots). This image shows the injection and subsequent breakup and evaporation of the liquid fuel. Following evaporation, the fuel vapor combusts, producing a lifted flame. The flame is stabilized due to the recirculation of hot gases in the center of the combustion chamber.

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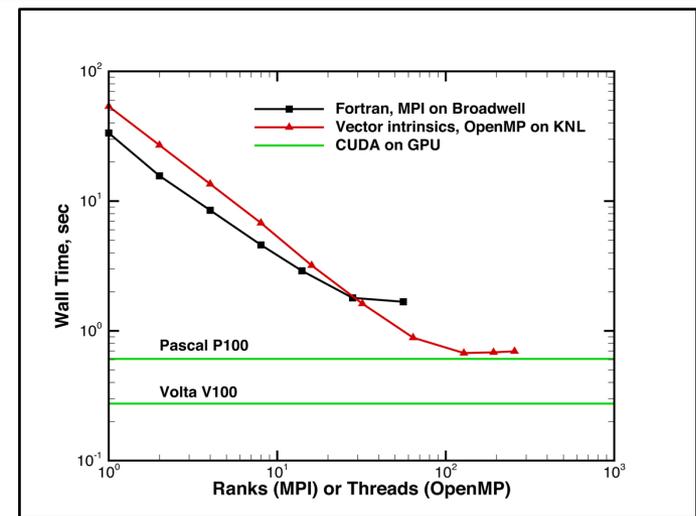
Developing New Algorithms for a Many-Core High-Performance Computing Landscape*



- The newest generation of many-core processors presents challenges for software developers, as legacy multi-core codes must be restructured to ensure good performance, especially at exascale.
- To help prepare NASA's FUN3D code for future HPC architectures, researchers at NASA Langley and Old Dominion University ran simulations on Broadwell and Xeon Phi Knights Landing (KNL) processors, and NVIDIA GPUs. Studies included:
 - Data layout strategies & programming models, such as explicit domain decomposition with message passing, shared-memory approaches based on compiler directives, and assembly-level techniques.
 - Impact on vectorization and memory performance.
- Results showed:
 - The GPU hardware accelerates matrix construction substantially; the KNL architecture benefits greatly from explicit prefetching and vectorization.
 - Where thread safety is required, a coloring approach outperforms OpenMP atomics on the KNL processors, while atomic operations excel on the GPUs.
- These studies will help software developers identify key programming strategies for optimizing code performance on the new architectures.

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

Mission Impact: Made possible by HECC resources, this work will ultimately enable more timely and cost-effective solutions for NASA, including crewed and uncrewed space missions and numerous aeronautics applications ranging from fixed-wing vehicles to rotorcraft and supersonic configurations.



Performance of the multicolor, point-implicit, linear solver used by NASA's FUN3D code on Pleiades Intel Xeon (Broadwell) and Xeon Phi (KNL) processors, and NVIDIA GPUs. Different programming models are used for each; the many-core architectures show a considerable speedup over the baseline Xeon hardware.

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HECC Facility Hosts Several Visitors and Tours in July 2018



- HECC hosted 15 tour groups in July; guests learned about the agency-wide missions being supported by HECC assets, and some groups also viewed the D-Wave 2000Q quantum computer system. Visitors this month included:
 - James Greene, NASA Chief Scientist.
 - Jack Kaye, Associate Director for Research of the Earth Science Division within NASA's Science Mission Directorate.
 - Pichet Durongkaverroj, Minister of Digital Economy and Society, Thailand.
 - The Honorable Julie Bishop MP, Minister of Foreign Affairs, Commonwealth of Australia, and her team.
 - 180 students and summer interns (8 large groups) from various universities and directorates at NASA Ames.



Piyush Mehrotra, Chief, NASA Advanced Supercomputing Division, gives a science demonstration on the hyperwall to the Honorable Julie Bishop MP, Minister of Foreign Affairs, Commonwealth of Australia (front row, middle) and her team; Ames Deputy Director, Carol Carroll is to the right of the Minister.

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



- **“Atmospheric Energy Deposition Modeling and Inference for Varied Meteoroid Structures,”** L. Wheeler, D. Mathias, E. Stokan, P. Brown, *Icarus*, vol. 315, published online June 28, 2018. *
<https://www.sciencedirect.com/science/article/pii/S0019103518301313?via%3Dihub>
- **“Non-Thermal X-Rays from Colliding Wind Shock Acceleration in the Massive Binary Eta Carinae,”** K. Hamaguchi, et al., *Nature Astronomy: Letters*, July 2, 2018. *
<https://www.nature.com/articles/s41550-018-0505-1>
- **“A Global Glacial Ocean State Estimate Constrained by Upper-Ocean Temperature Proxies,”** D. Amrhein, et al., *Journal of Climate*, published online July 5, 2018. *
<https://journals.ametsoc.org/doi/abs/10.1175/JCLI-D-17-0769.1>
- **“Sparse Wavefront Control: A New Approach to High-Contrast Imaging,”** E. Bendek, D. Sirbu, C. Henze, et al., *Proceedings Volume 10698, Space Telescopes and Instrumentation: Optical, Infrared, and Millimeter Wave*, July 6, 2018. *
<https://www.spiedigitallibrary.org/conference-proceedings-of-spie/10698/106981M/Sparse-wavefront-control--A-new-approach-to-high-contrast/10.1117/12.2313963.short?SSO=1>
- **“Multi-Star Wavefront Control for the Wide-Field Infrared Survey Telescope Coronagraph Instrument,”** D. Sirbu, R. Belikov, E. Bendeck, C. Henze, et al., *Proceedings Volume 10698, Space Telescopes and Instrumentation: Optical, Infrared, and Millimeter Wave*, July 6, 2018. *
<https://www.spiedigitallibrary.org/conference-proceedings-of-spie/10698/106982F/Multi-star-wavefront-control-for-the-Wide-Field-Infrared-Survey/10.1117/12.2314145.short?SSO=1>

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



- **AIAA/SAE/ASME Joint Propulsion Conference**, Cincinnati, OH, July 9–11, 2018.
 - **“Evaluation of Turbulent Combustion Models for Canonical Premixed/Non-Premixed Combustors,”** K. Miki, J. Moder, T. Wey, M.-S. Liou. *
<https://arc.aiaa.org/doi/abs/10.2514/6.2018-4919>
 - **“Effect of Chemistry Modeling on Flame Stabilization of a Swirl Spray Combustor,”** A. Panchal, et al. *
<https://arc.aiaa.org/doi/abs/10.2514/6.2018-4684>
 - **“Comparison of Mixing Characteristics for Several Fuel Injectors at Mach 8 and 15 Hypervelocity Flow Conditions,”** R. Shenoy, T. Droza, A. Norris, R. Baurle, J. Drummond. *
<https://arc.aiaa.org/doi/abs/10.2514/6.2018-4540>
 - **“Subgrid-Scale Modeling for Large Eddy Simulations of Dense-to-Dilute Multiphase Reacting Flows,”** A. Panchal, R. Ranjan, S. Menon. *
<https://arc.aiaa.org/doi/abs/10.2514/6.2018-4733>
 - **“Computational Study of Compact Ejector-Enhanced Resonant Pulse Combustors,”** S. Yungster, et al. *
<https://arc.aiaa.org/doi/abs/10.2514/6.2018-4786>
 - **“Numerical Simulation of Flow Distribution in a Realistic Gas Turbine Combustor,”** V. Hasti, et al. *
<https://arc.aiaa.org/doi/abs/10.2514/6.2018-4956>
 - **“Numerical Study of the Detonation Wave Structure in a Linear Model Detonation Engine,”** S. Prakash, R. Fievet, V. Raman, J. Burr, K. Yu. *
<https://arc.aiaa.org/doi/abs/10.2514/6.2018-4966>
- **“Validating Forward Modeling and Inversions of Helioseismic Holography Measurements,”** K. DeGrave, et al., arXiv:1807.03841 [astro-ph.SR], July 10, 2018. *
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* HECC provided supercomputing resources and services in support of this work



- **“Generating High Resolution Climate Change Projections through Single Image Super-Resolution: An Abridged Version,”** T. Vandal, et al., Proceedings of the Twenty-Seventh International Joint Conference on Artificial Intelligence, Stockholm, Sweden, July 13–19, 2018. *
<https://www.ijcai.org/proceedings/2018/0759.pdf>
- **“Big Data and Extreme-Scale Computing,”** M. Asch, T. Moore, R. Badia, et al., The International Journal of High Performance Computing Applications, July 16, 2018. *
<http://journals.sagepub.com/doi/abs/10.1177/1094342018778123>
- **“The VIMOS Public Extragalactic Redshift Survey (VIPERS): Unbiased Clustering Estimate with VIPERS Slit Assignment,”** F. Mohammad, D. Bianchi, W. Percival, et al., arXiv:1807.05999 [astro-ph.CO], July 16, 2018. *
<https://arxiv.org/abs/1807.05999>
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- **“Simulating an Isolated Dwarf Galaxy with Multi-Channel Feedback and Chemical Yields from Individual Stars,”** A. Emerick, et al., arXiv:1807.07182 [astro-ph.GA], July 18, 2018. *
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- **“Coupling of Turbulence on the Ignition of Multicomponent Sprays,”** P. Govindaraju, T. Jaravel, M. Ihme, Proceedings of the Combustion Institute (Elsevier), July 18, 2018. *
<https://www.sciencedirect.com/science/article/pii/S154074891830172X>
- **“Are Extreme Dissipation Events Predictable in Turbulent Fluid Flows?”** P. Blonigan, M. Farazmand, T. Sapsis, arXiv:1807.10263 [physics.flu-dyn], July 26, 2018. *
<https://arxiv.org/abs/1807.10263>

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Presentations

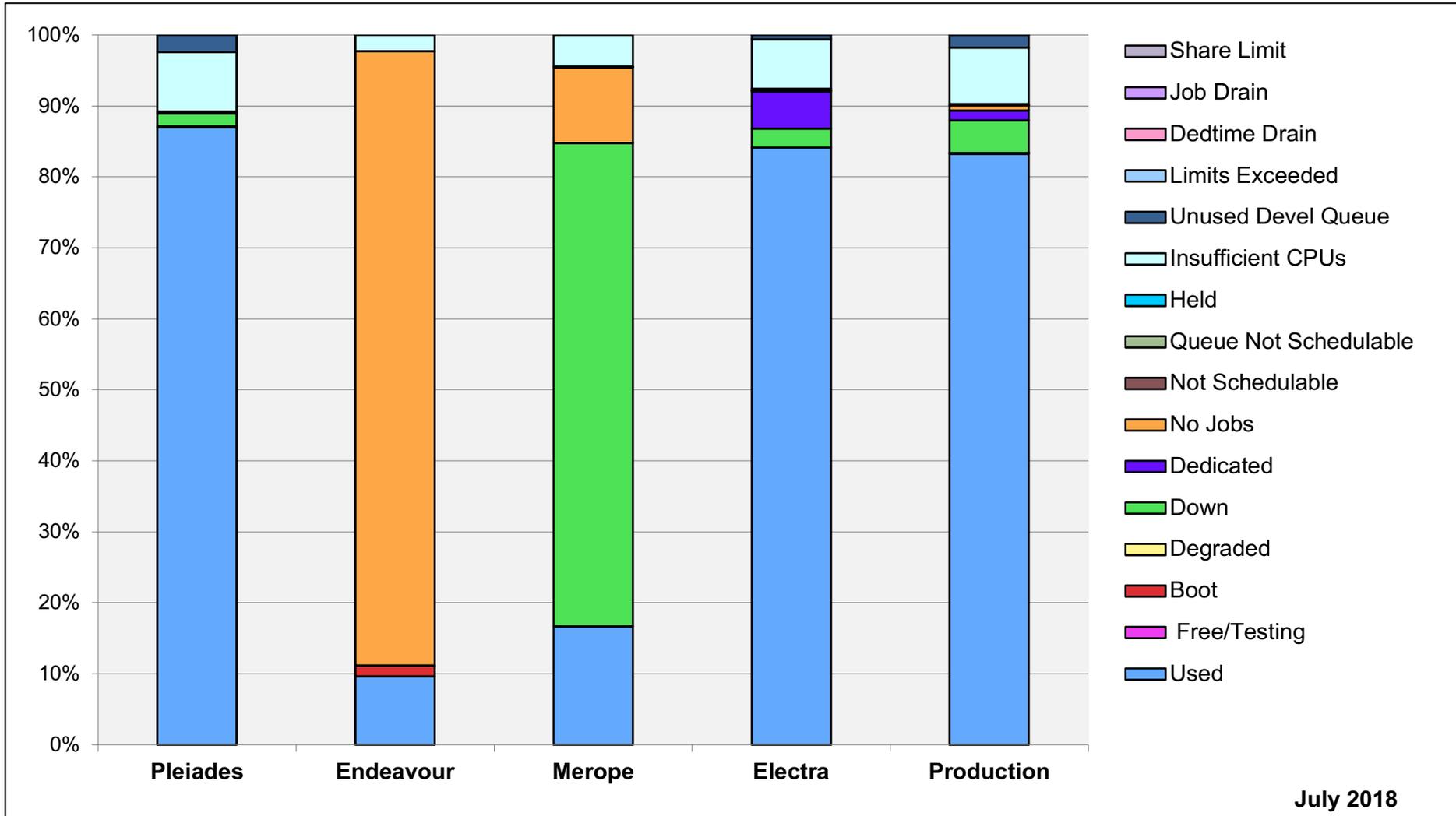


- **“Uncertainty and A-Posteriori Error Bound Estimates for General CFD Calculations,”** T. Barth, presented at the Platform for Advanced Scientific Computing (PASC) 2018 Conference, Basel, Switzerland, July 2-4, 2018.
- **Tenth International Conference on Computational Fluid Dynamics (ICCFD10)**, Barcelona, Spain, July 9–13, 2018.
 - **“An Automated Marching Scheme for Overset Structured Surface Mesh Generation,”** S. Pandya, W. Chan, R. Haimes.
<http://www.iccfd.org/iccfd10/papers/ICCFD10-097-Paper.pdf>
 - **“Performance Enhancements for the Lattice-Boltzmann Solver in the LAVA Framework,”** M. Barad, J. Jocheemoolayil, G. Stich, C. Kiris.
<http://www.iccfd.org/iccfd10/papers/ICCFD10-101-Paper.pdf>
 - **“Numerical Simulation of Dynamic Stall Using Near-Body Adaptive Mesh Refinement,”** N. Chaderjian.
<http://www.iccfd.org/iccfd10/papers/ICCFD10-102-Paper.pdf>
 - **“Validation of WMLES on a Periodic Channel Flow Featuring Adverse/Favorable Pressure Gradients,”** C. Carton de Wiart, J. Larsson, S. Murman.
<http://www.iccfd.org/iccfd10/papers/ICCFD10-355-Paper.pdf>
- **“Progress in Accuracy and Stability Improvement of Nonlinear Filter Methods for Long Time Integration of Compressible Flows,”** H. Yee, invited speaker at the International Conference on Spectral and Higher Order Methods (ICOSAHOM 2018), London, England, July 9–13, 2018.



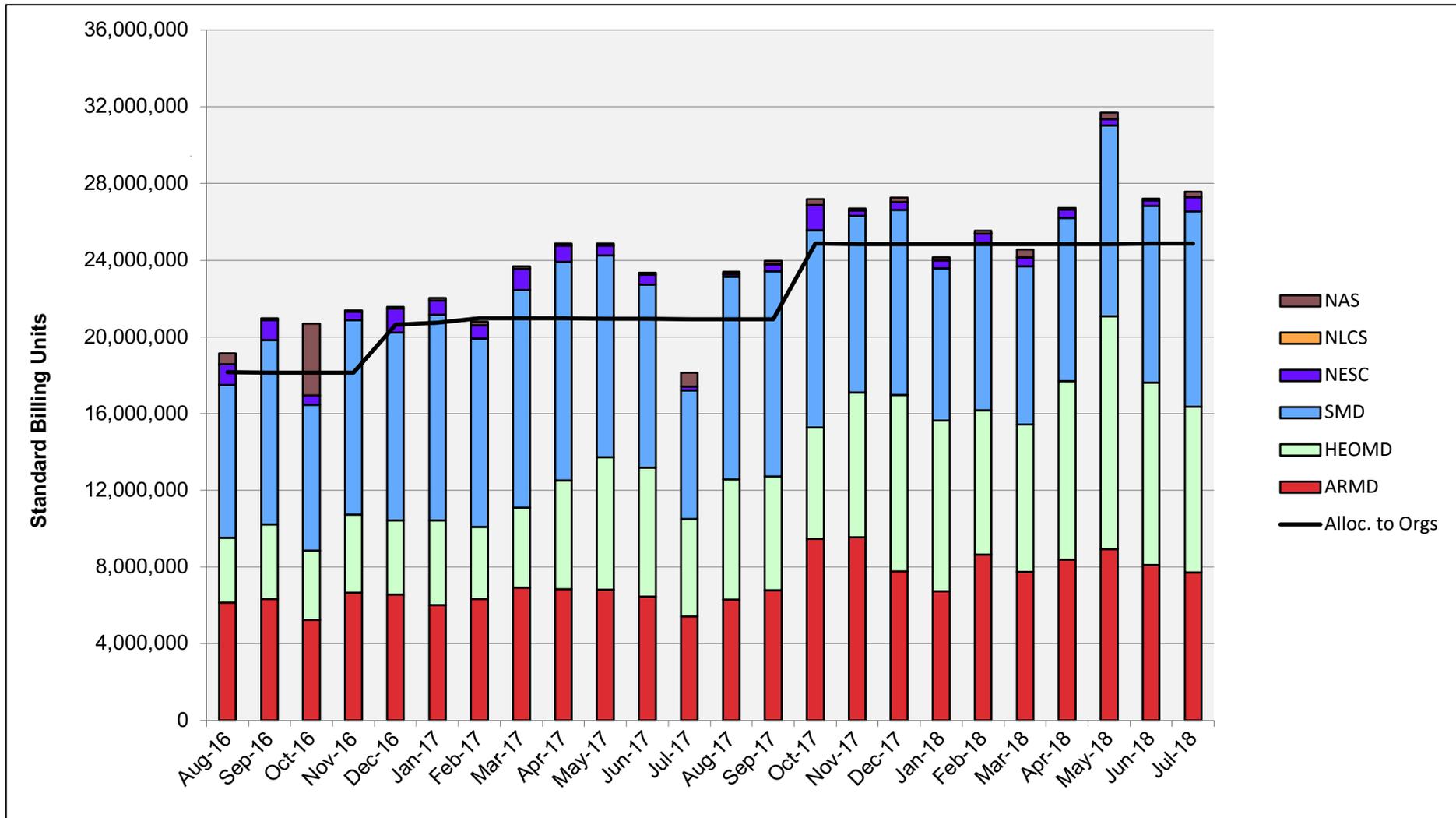
- **A Little Mixing Goes a Long Way: Breakthroughs in Simulating Tides' Impacts on Global Ocean Circulation**, *R&D*, July 19, 2018—Recent research is allowing scientists at NASA JPL to gain better insight of small-scale effects on our key planetary systems and helping them plan new satellite missions, running simulations on large supercomputers, like Pleiades and Electra at NASA Ames in California.
<https://www.rdmag.com/article/2018/07/little-mixing-goes-long-way-breakthroughs-simulating-tides-impacts-global-ocean-circulation>

HECC Utilization

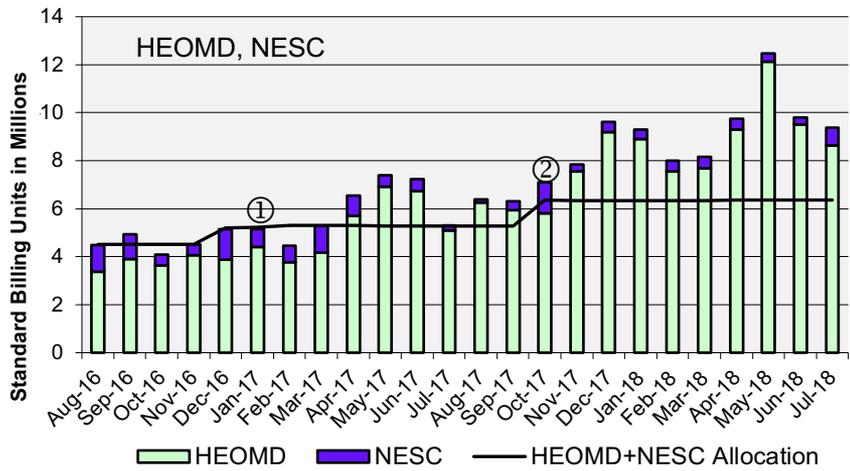
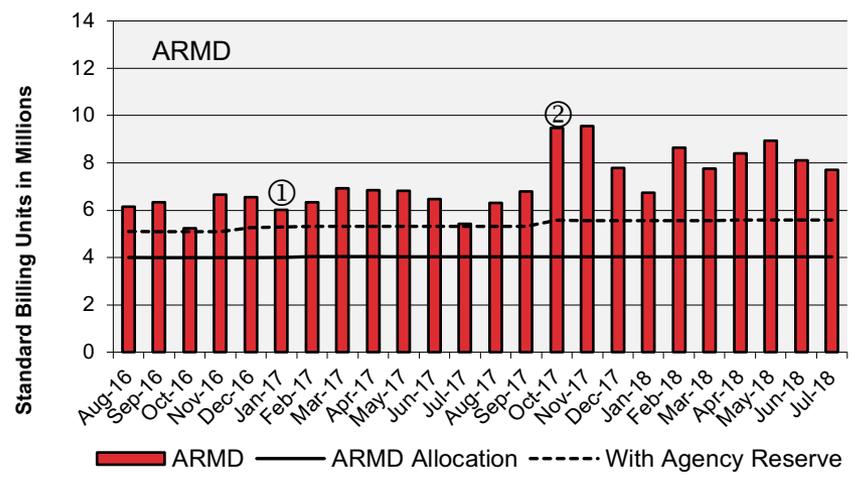
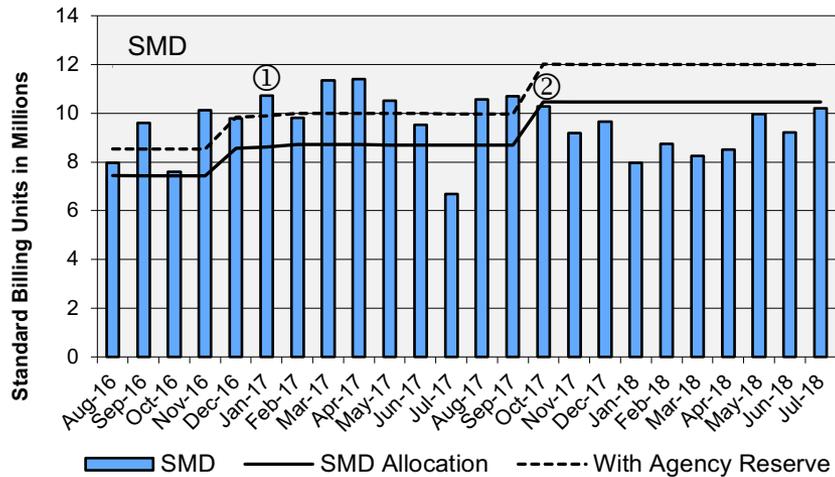


July 2018

HECC Utilization Normalized to 30-Day Month

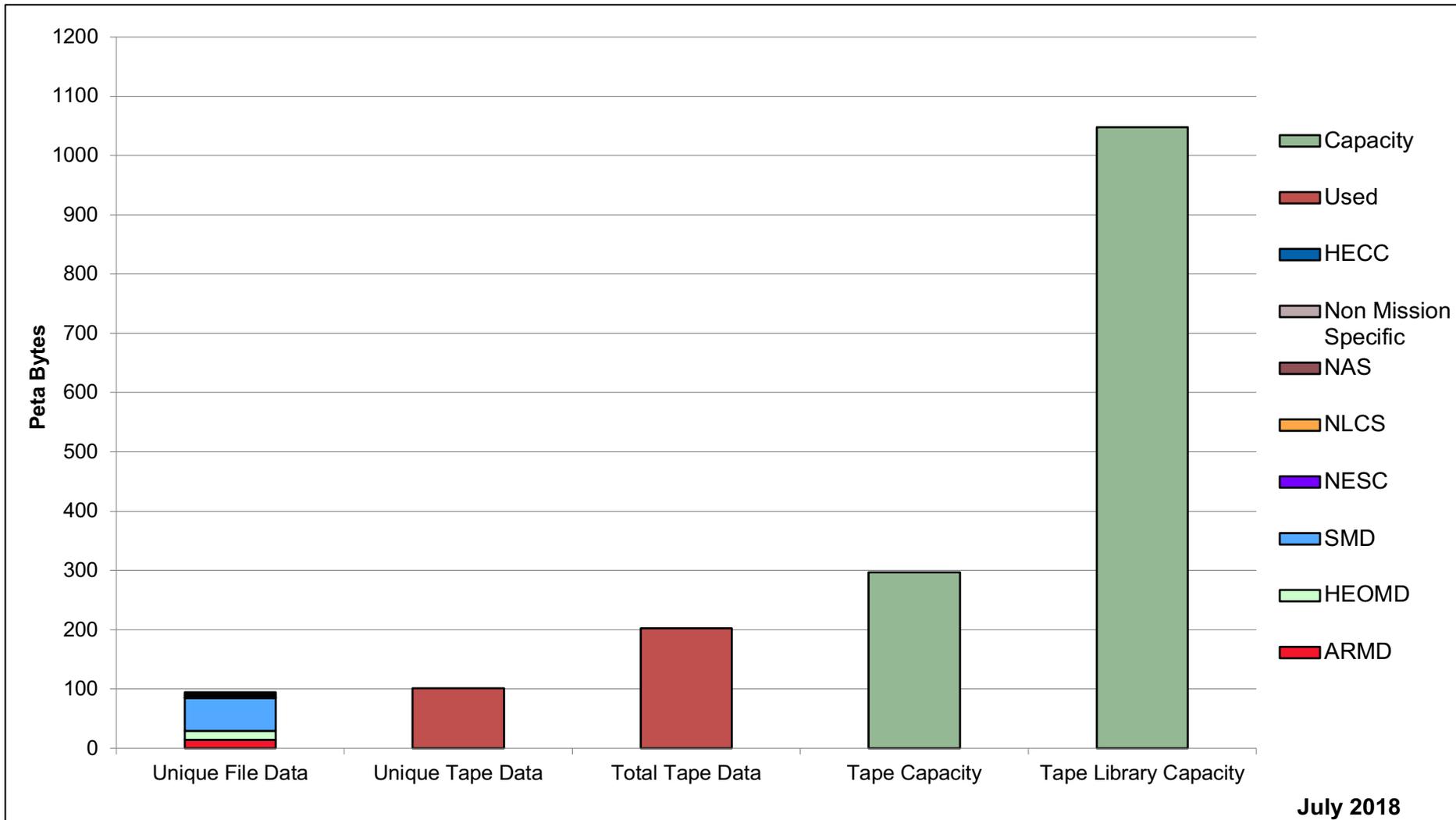


HECC Utilization Normalized to 30-Day Month

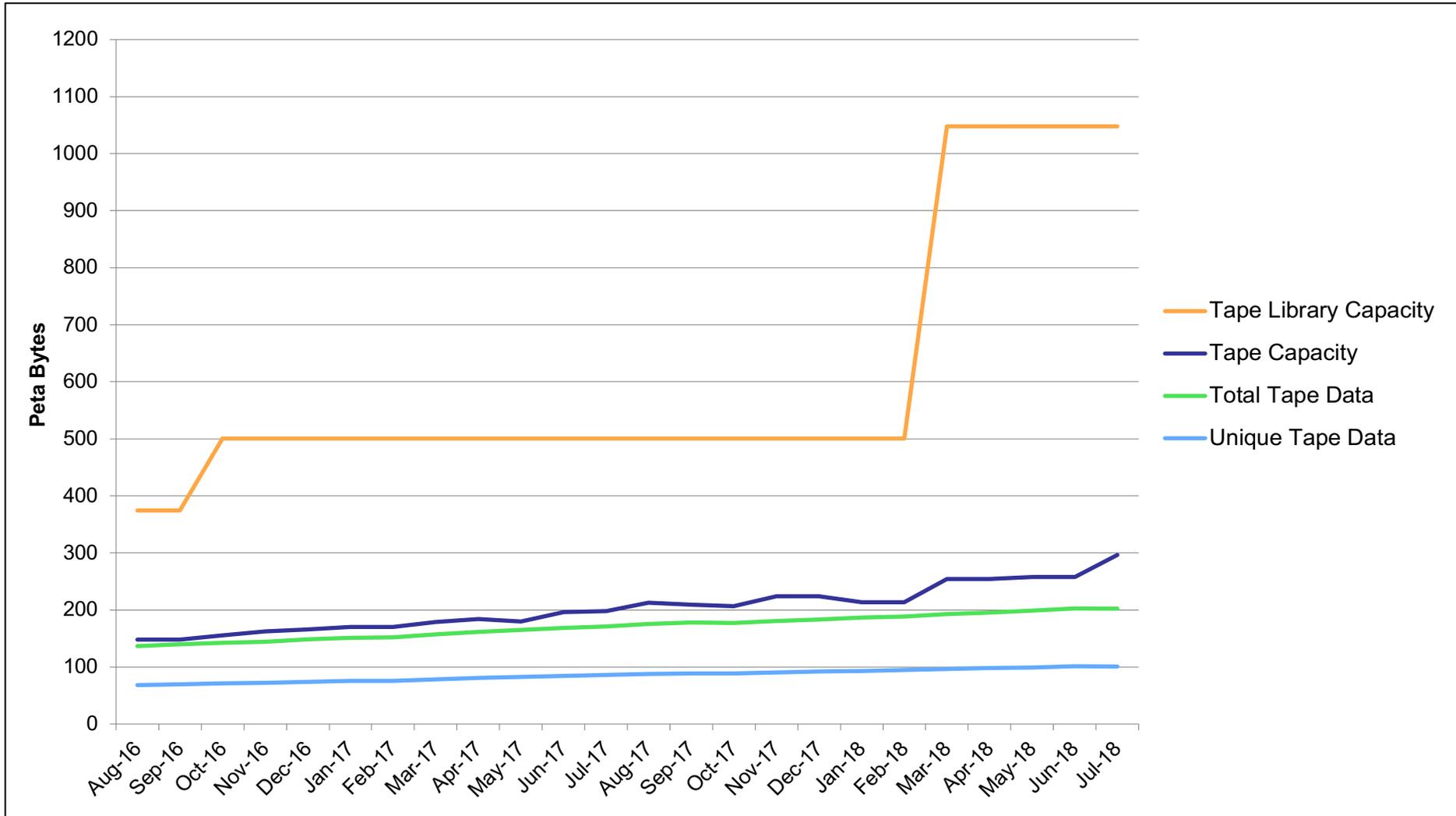


- ① 16 Broadwell racks added to Electra, 20 Westmere half racks added to Merope
- ② 4 Skylake E cells (16 D Rack Equivalence) added to Electra

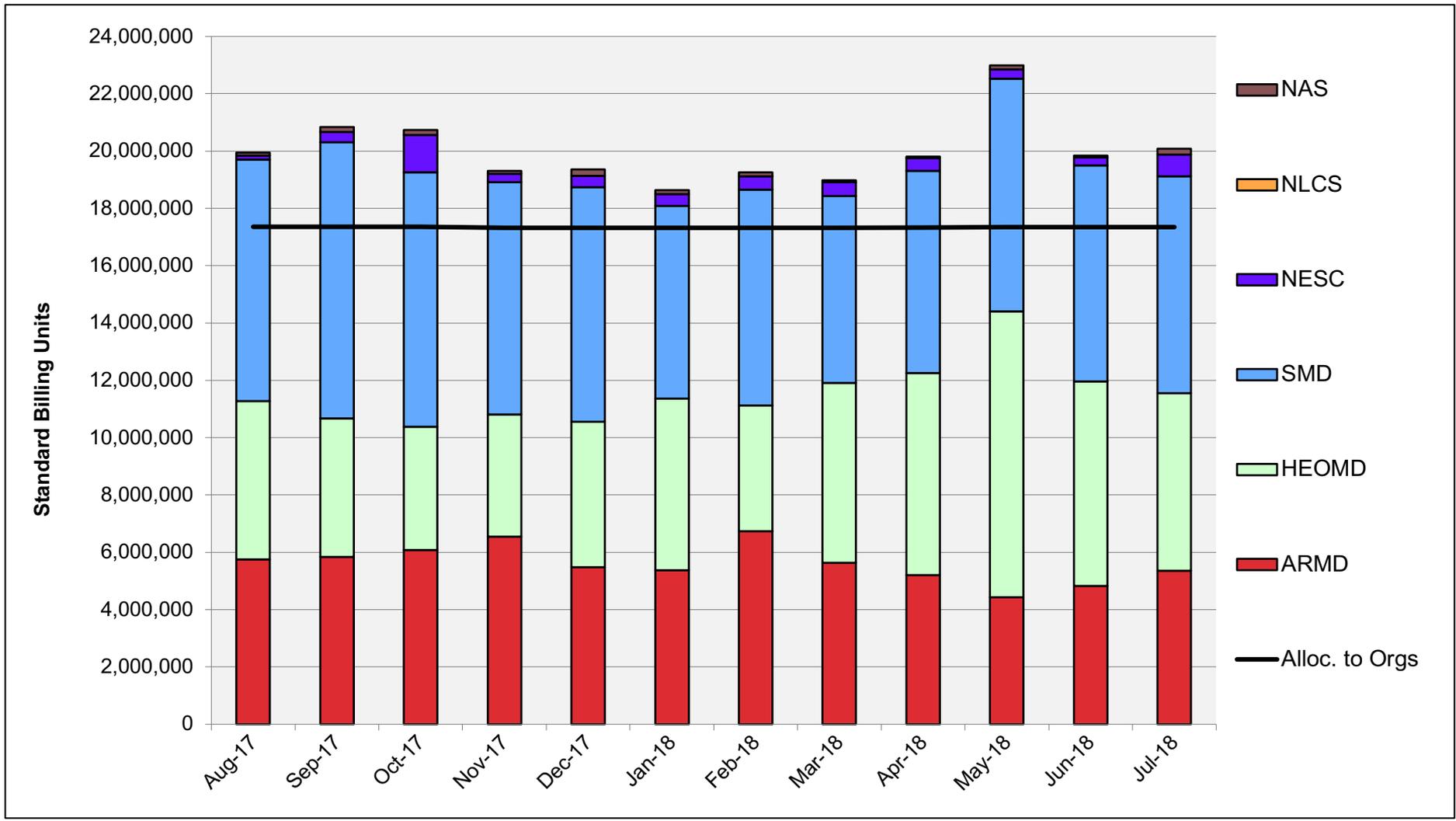
Tape Archive Status



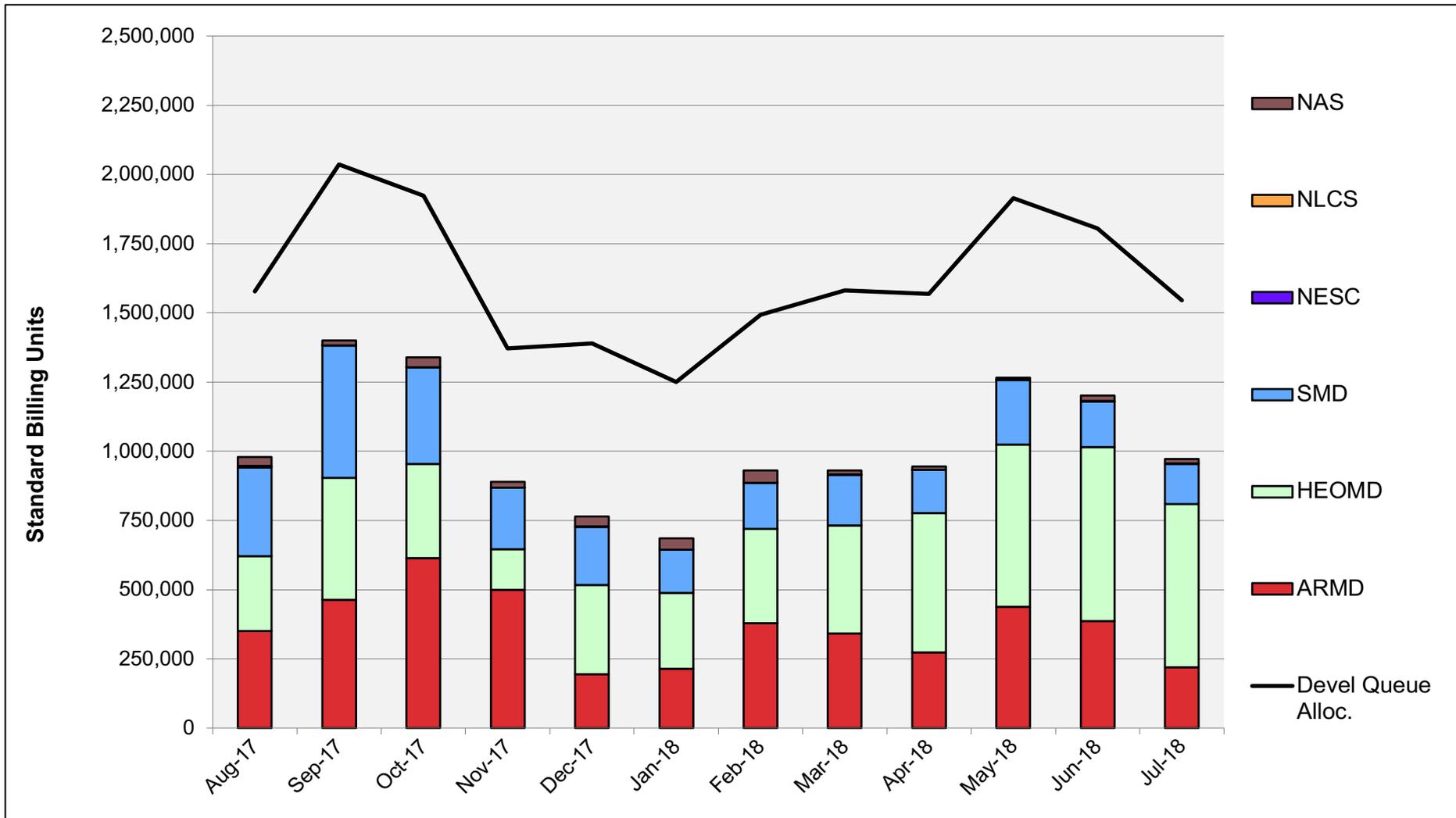
Tape Archive Status



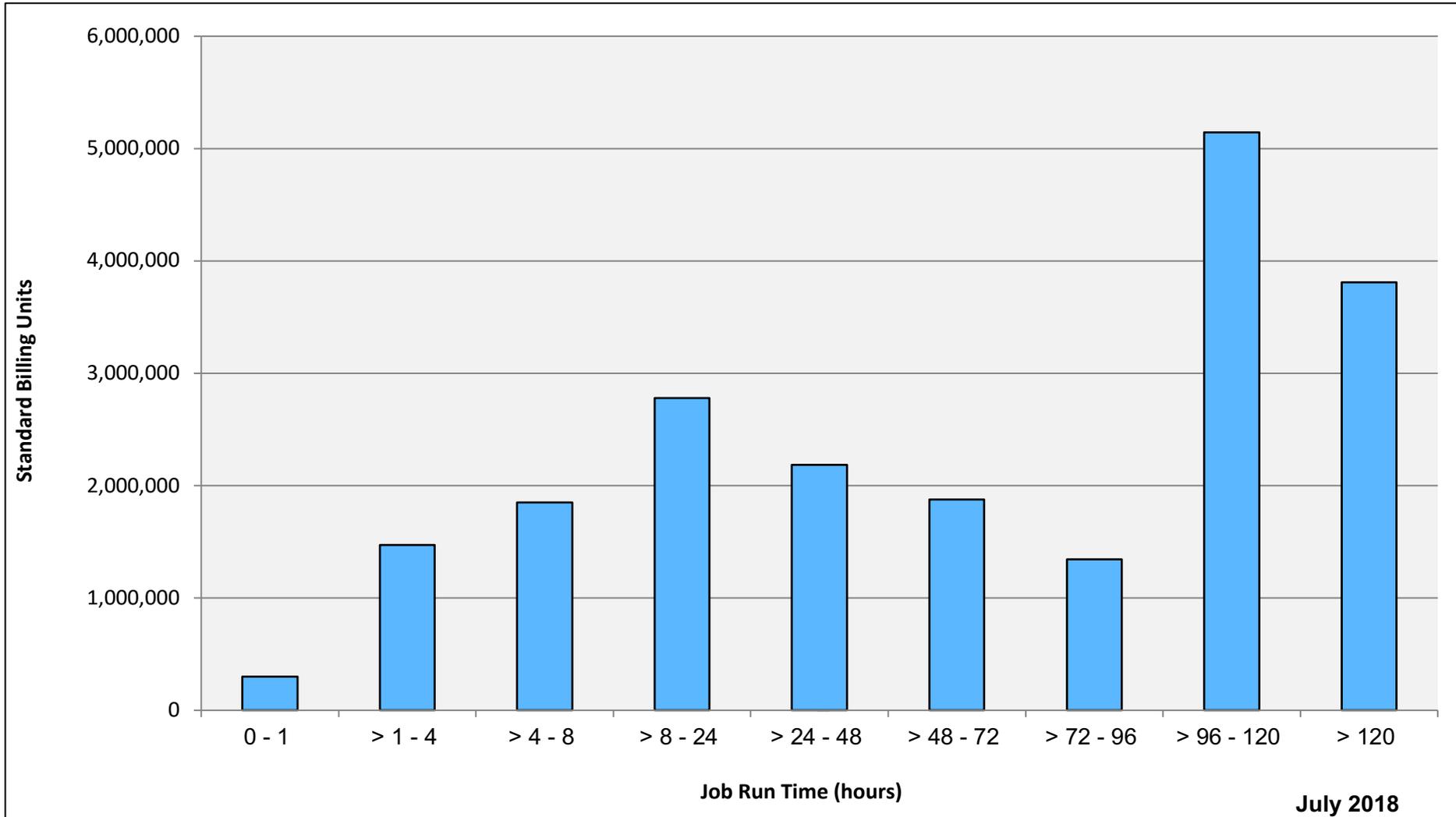
Pleiades: SBUs Reported, Normalized to 30-Day Month



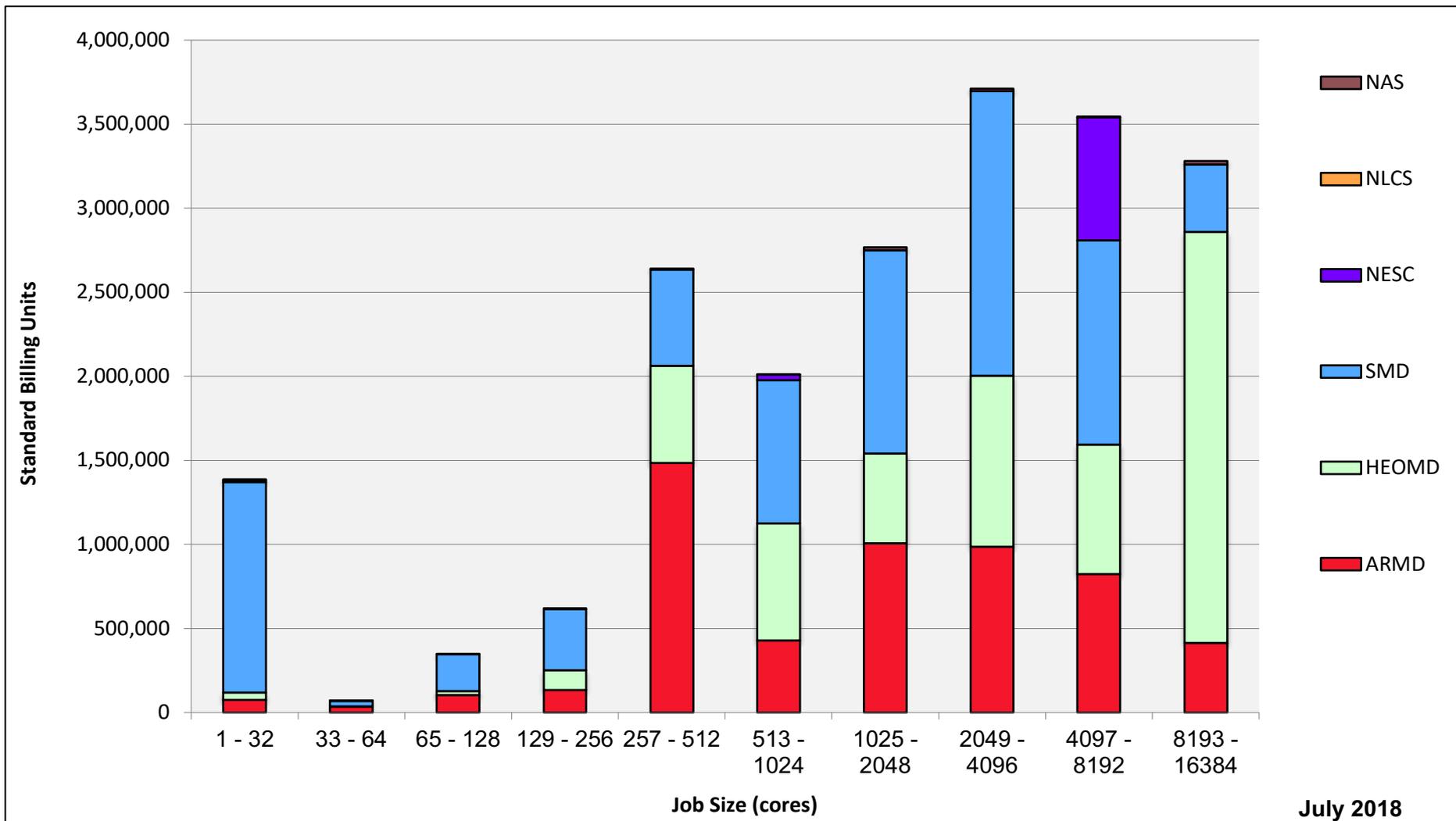
Pleiades: Devel Queue Utilization



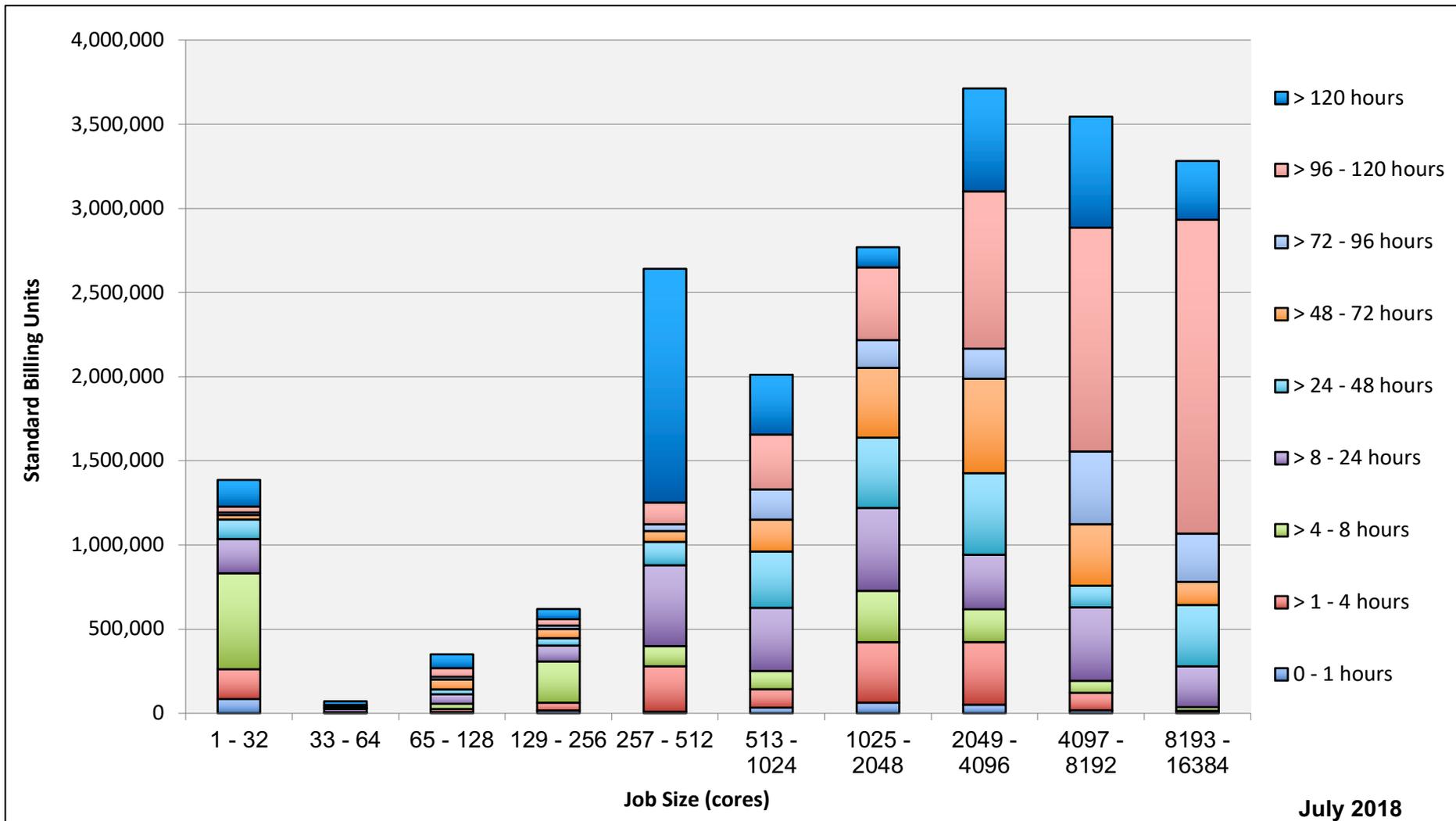
Pleiades: Monthly Utilization by Job Length



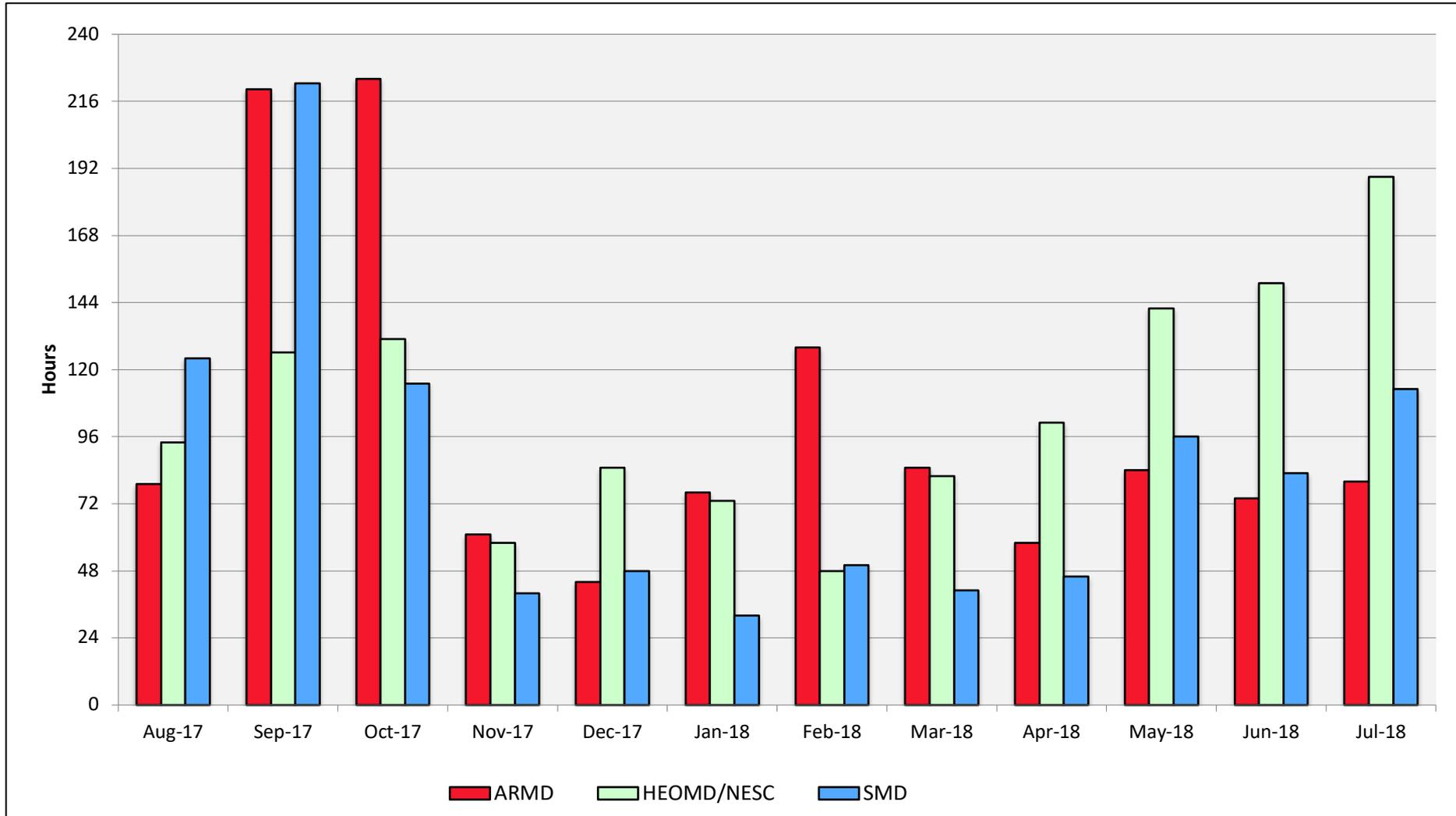
Pleiades: Monthly Utilization by Size and Mission



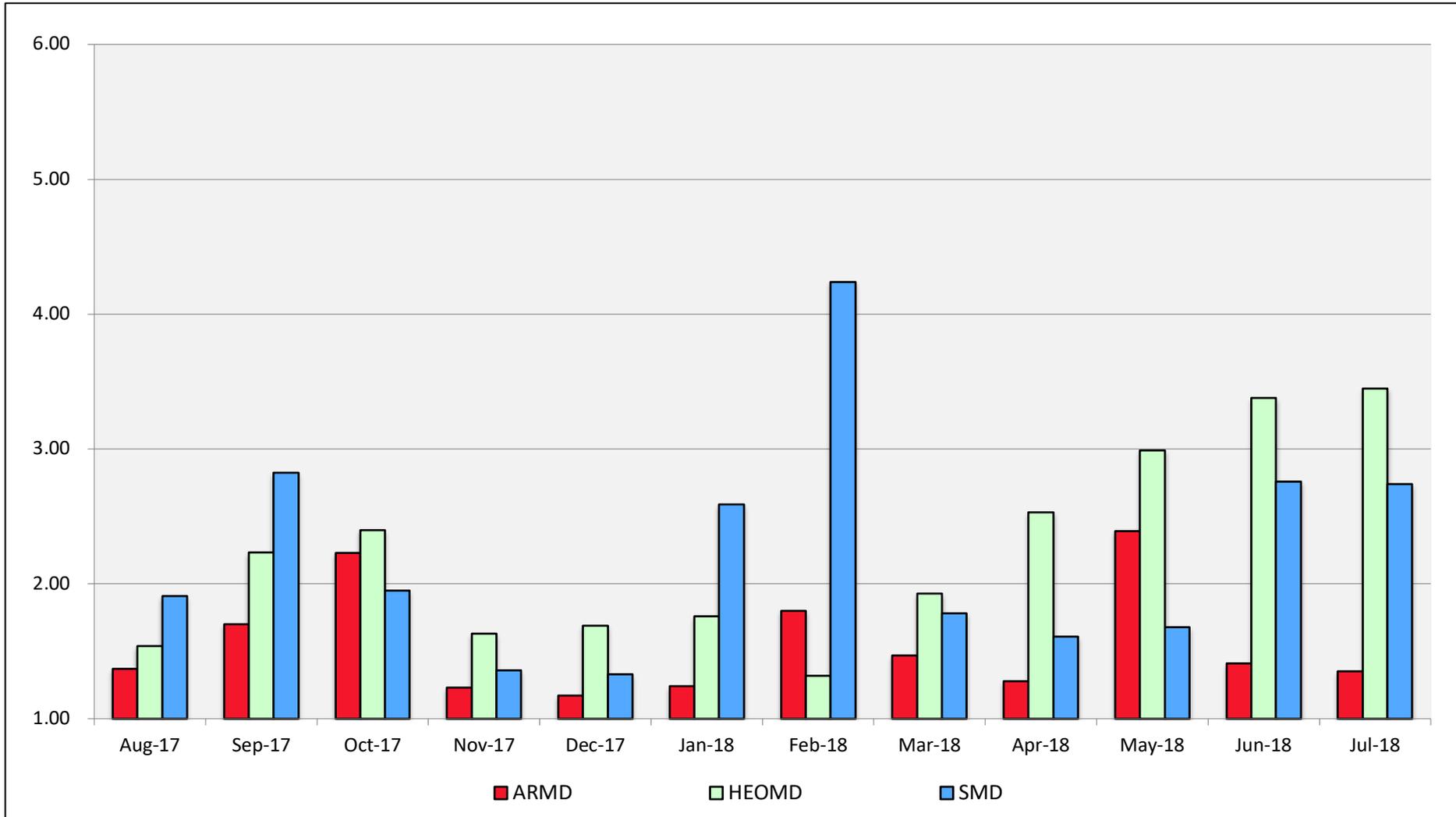
Pleiades: Monthly Utilization by Size and Length



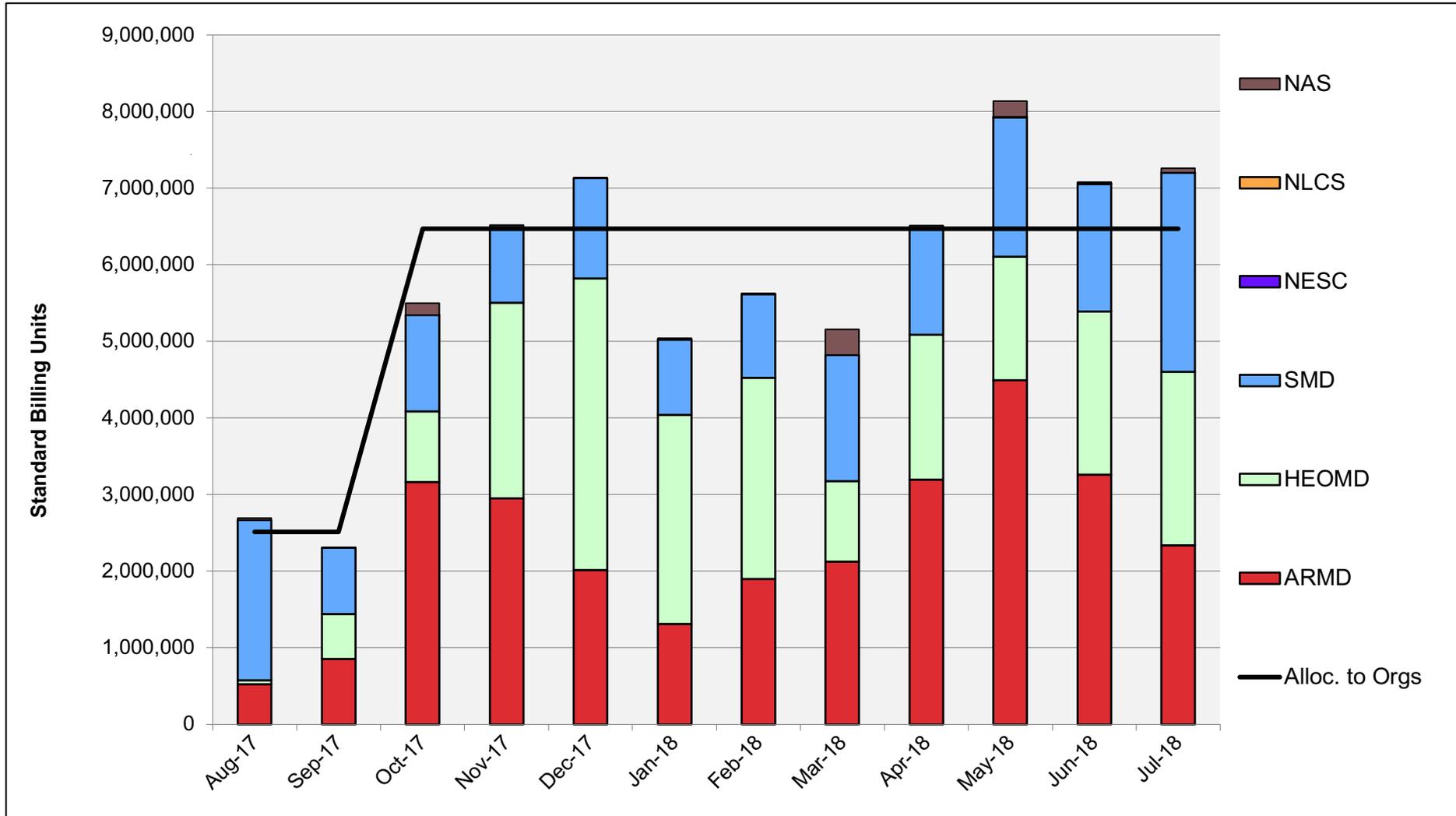
Pleiades: Average Time to Clear All Jobs



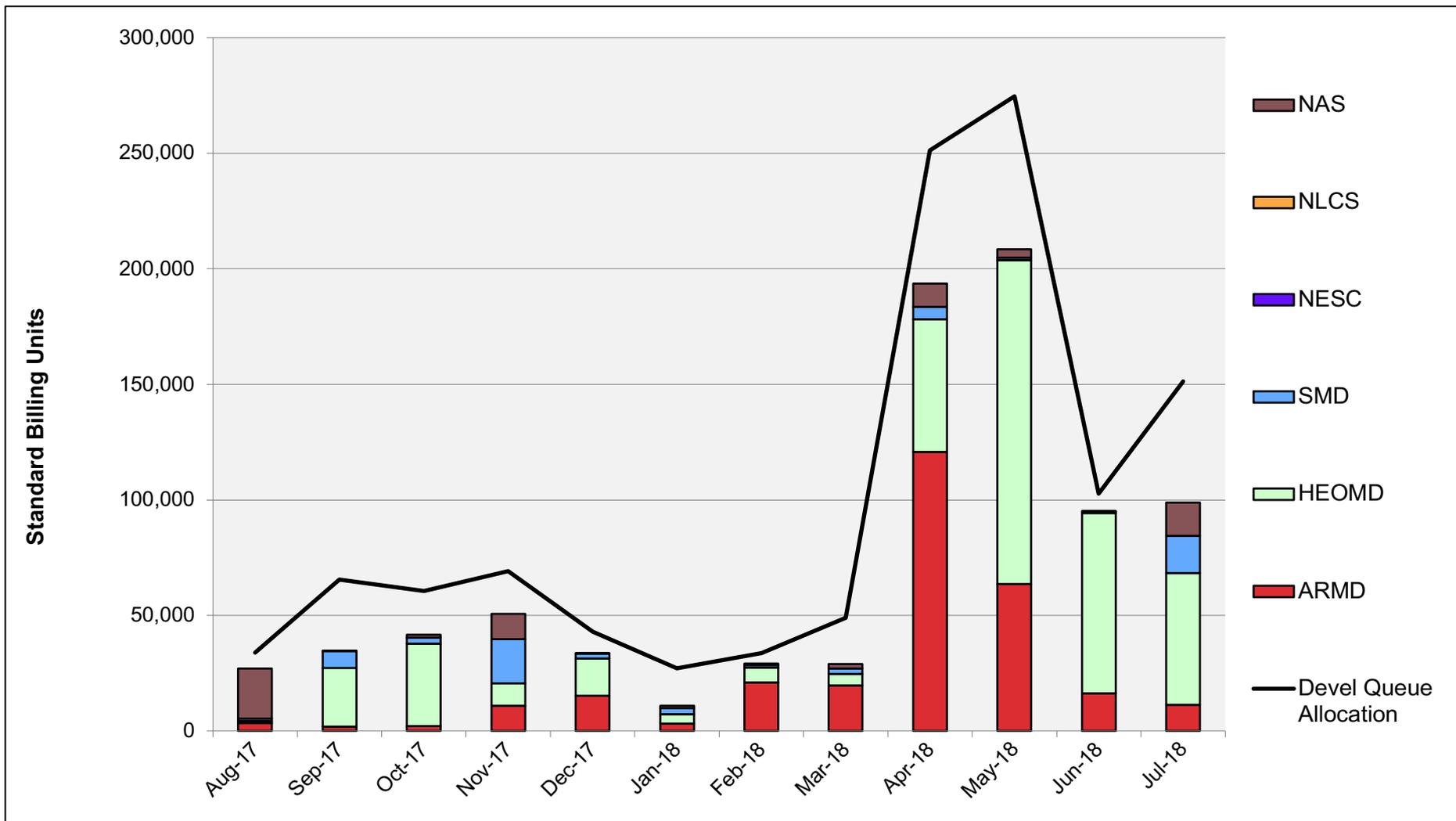
Pleiades: Average Expansion Factor



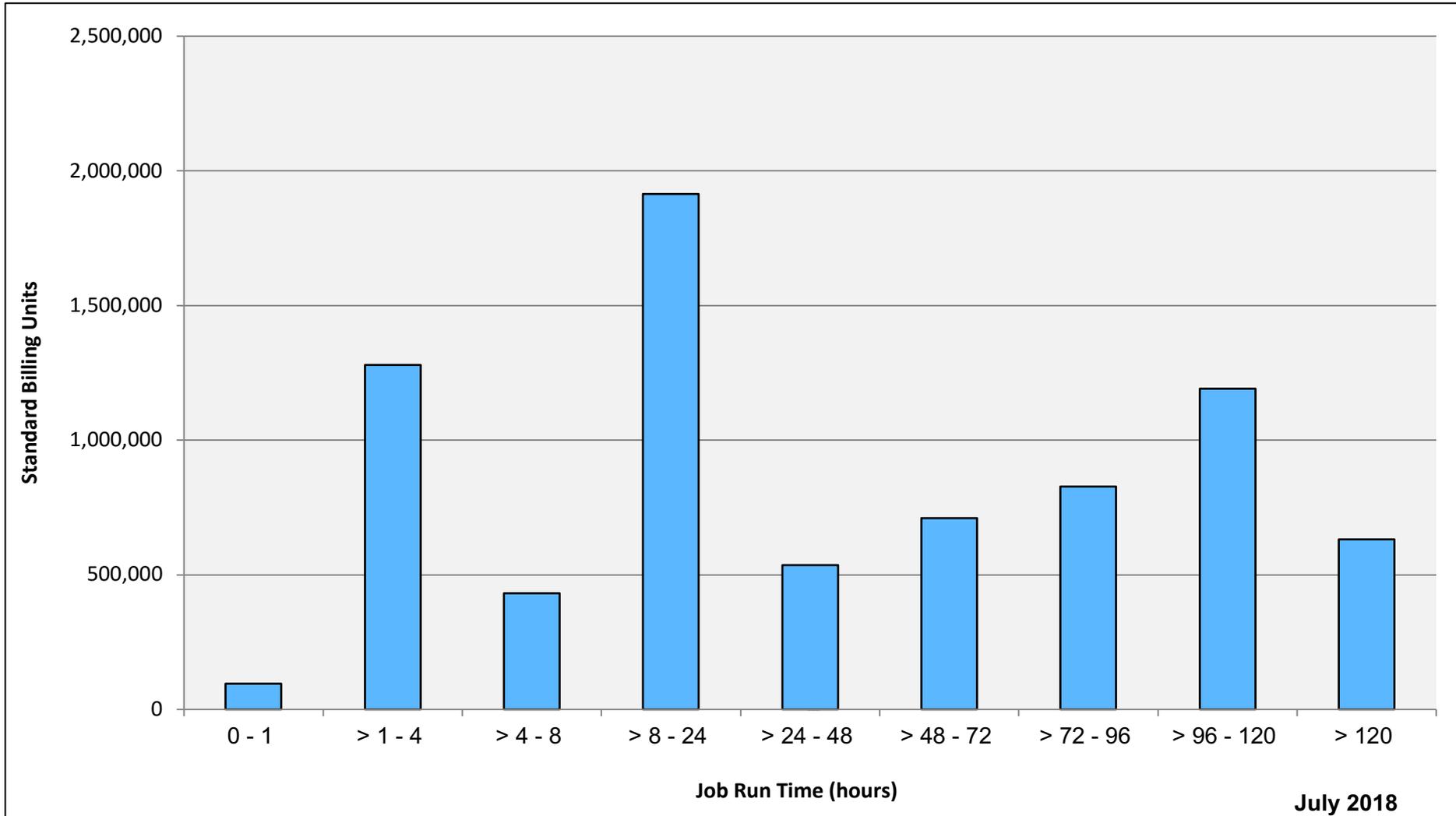
Electra: SBUs Reported, Normalized to 30-Day Month



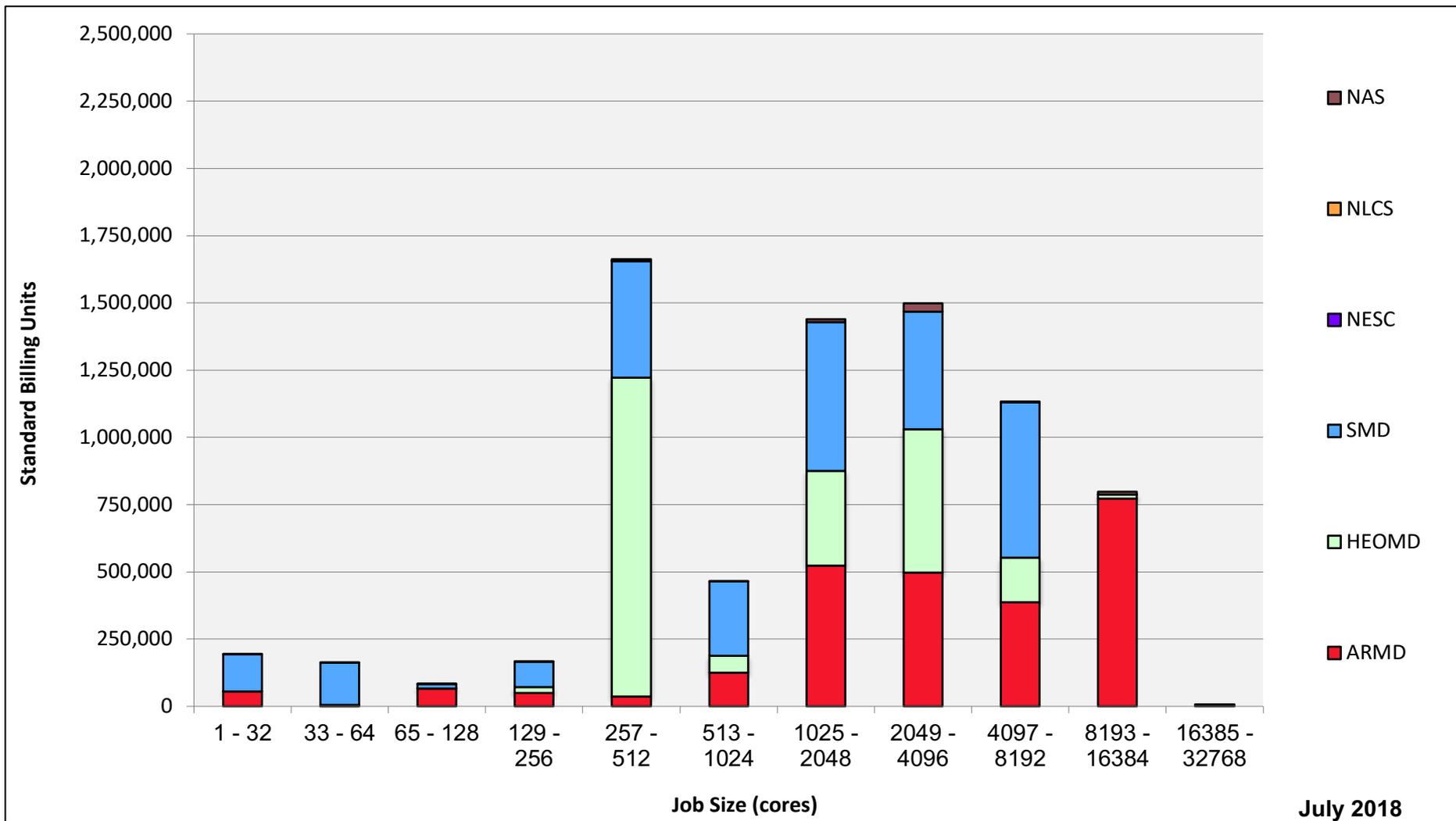
Electra: Devel Queue Utilization



Electra: Monthly Utilization by Job Length

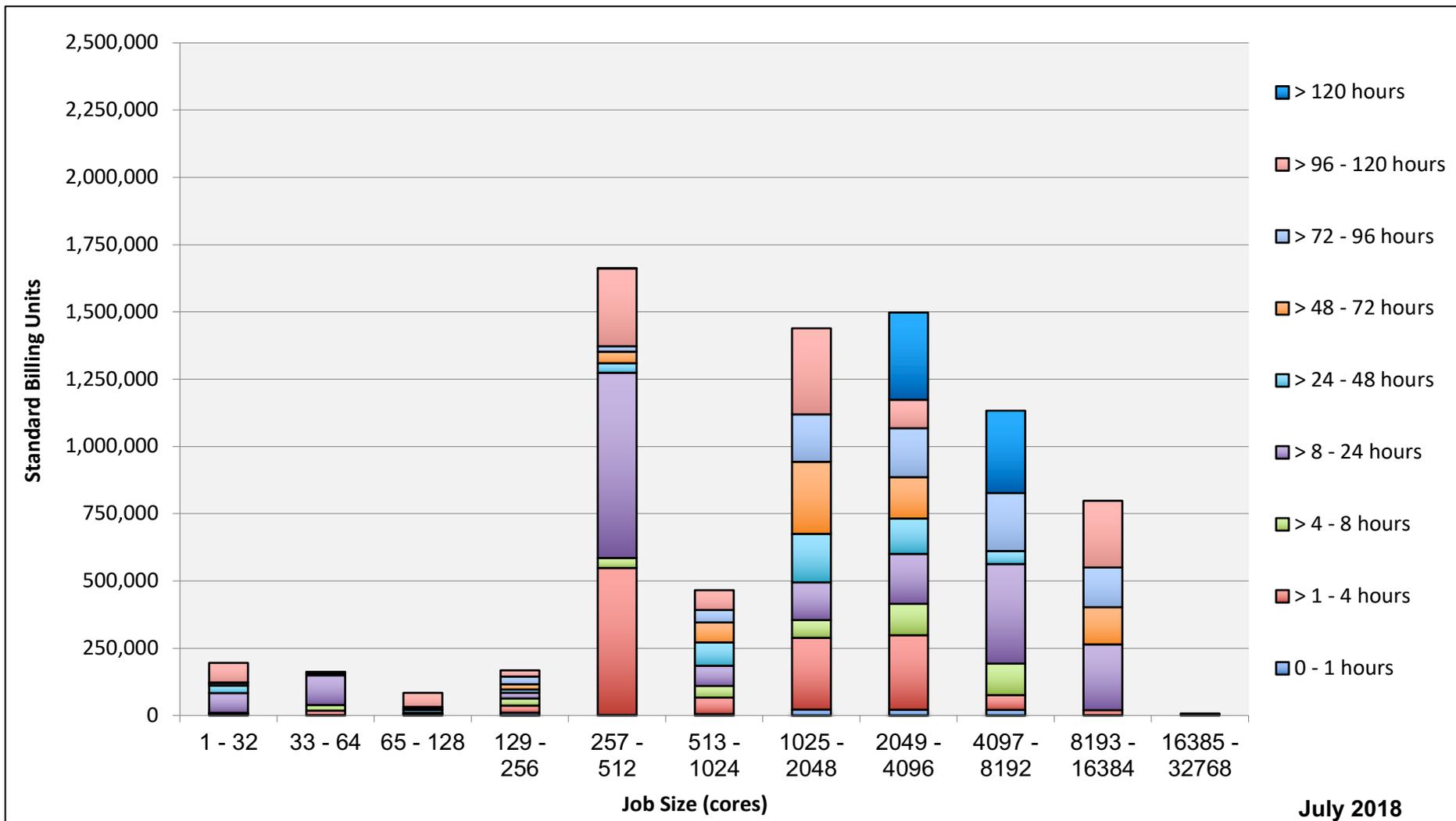


Electra: Monthly Utilization by Size and Mission



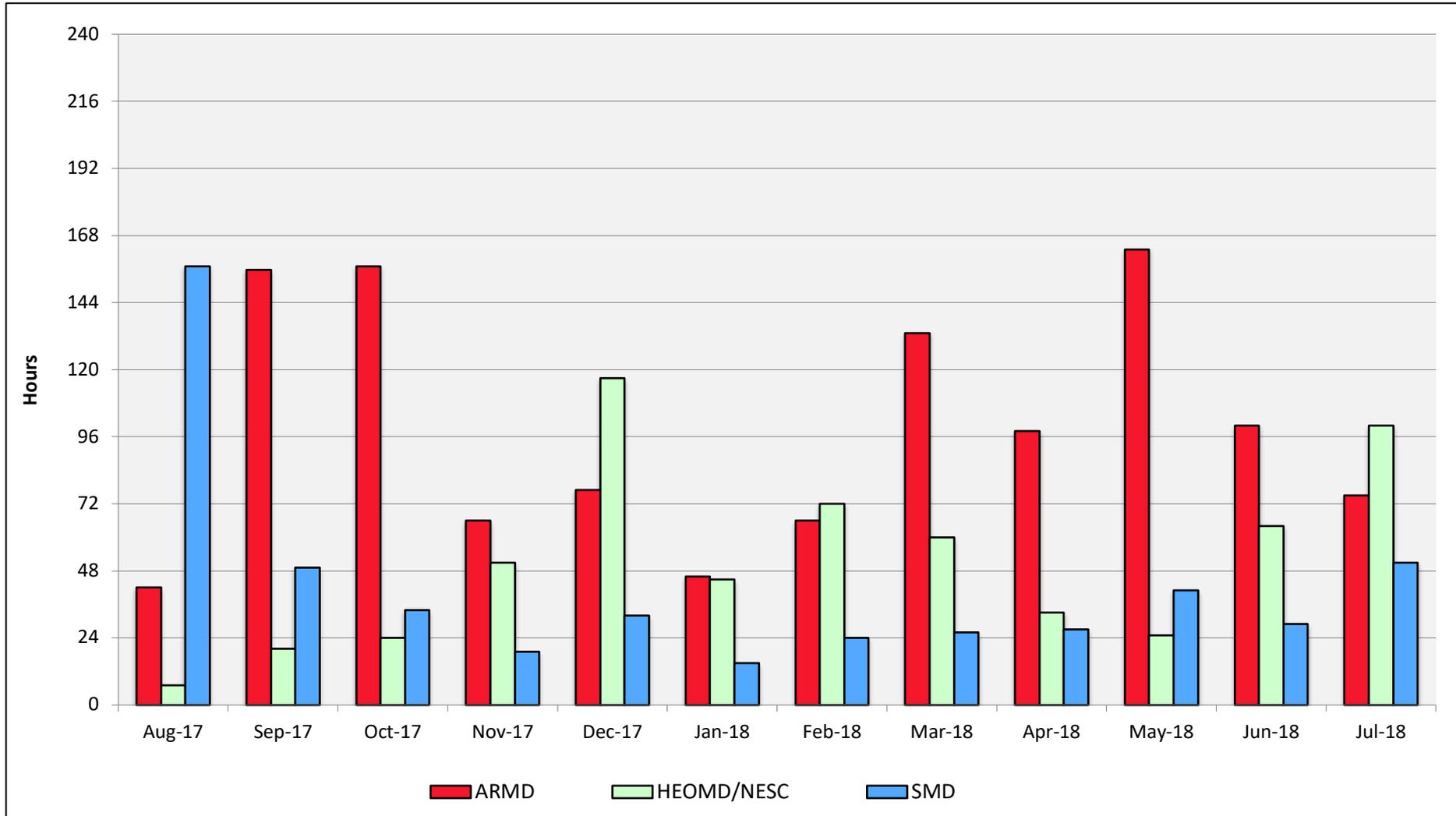
July 2018

Electra: Monthly Utilization by Size and Length

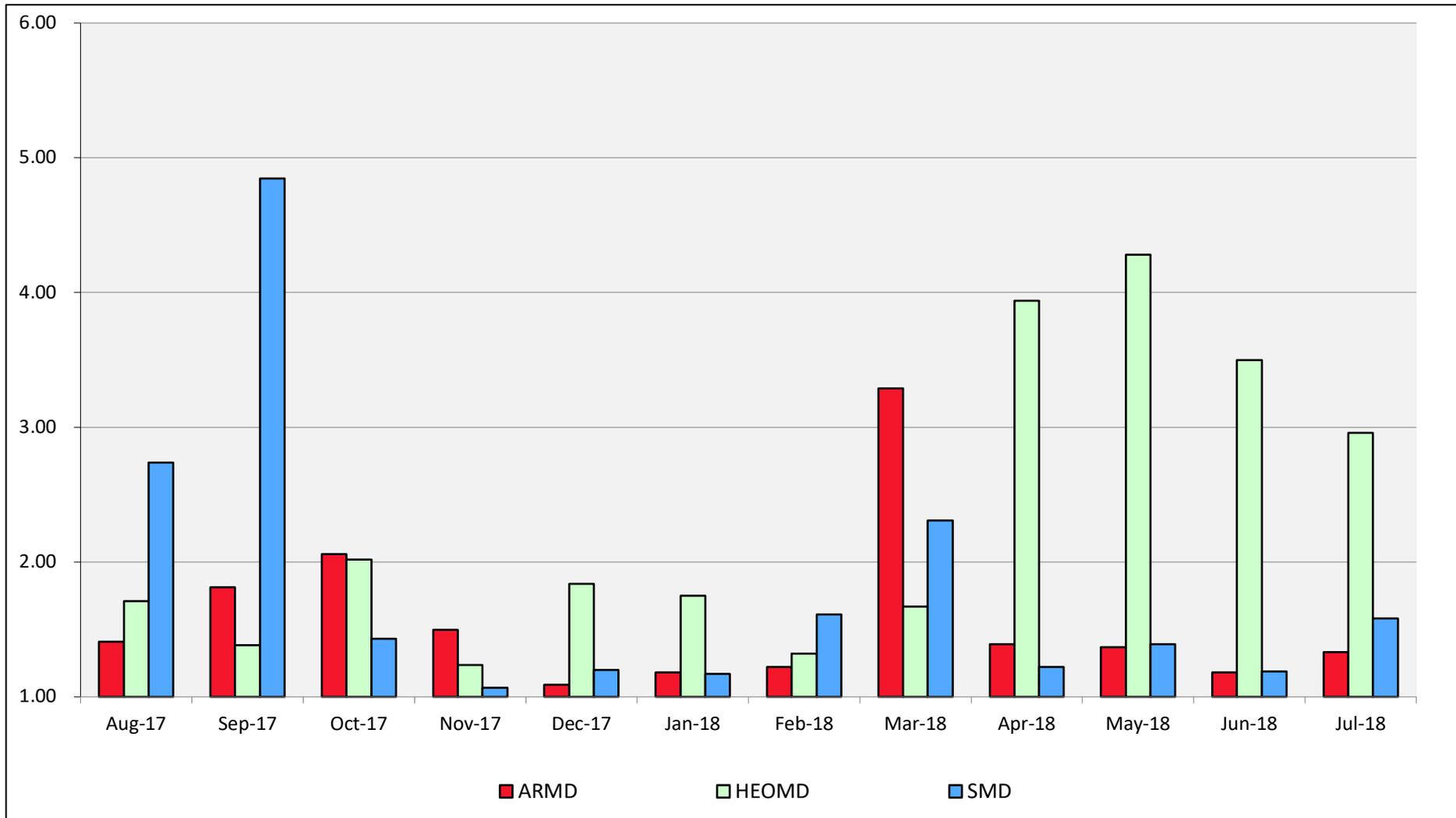


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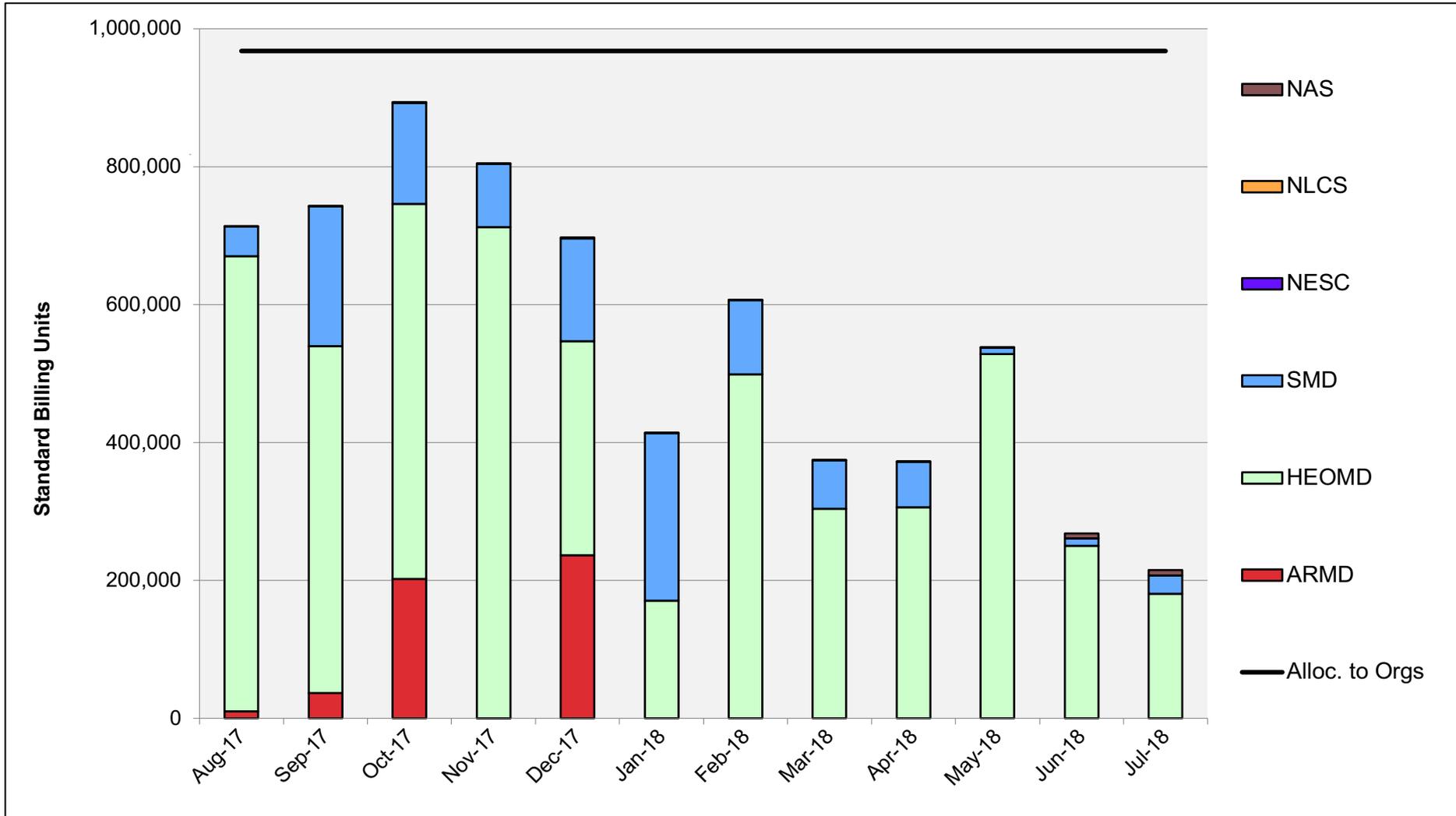
Electra: Average Time to Clear All Jobs



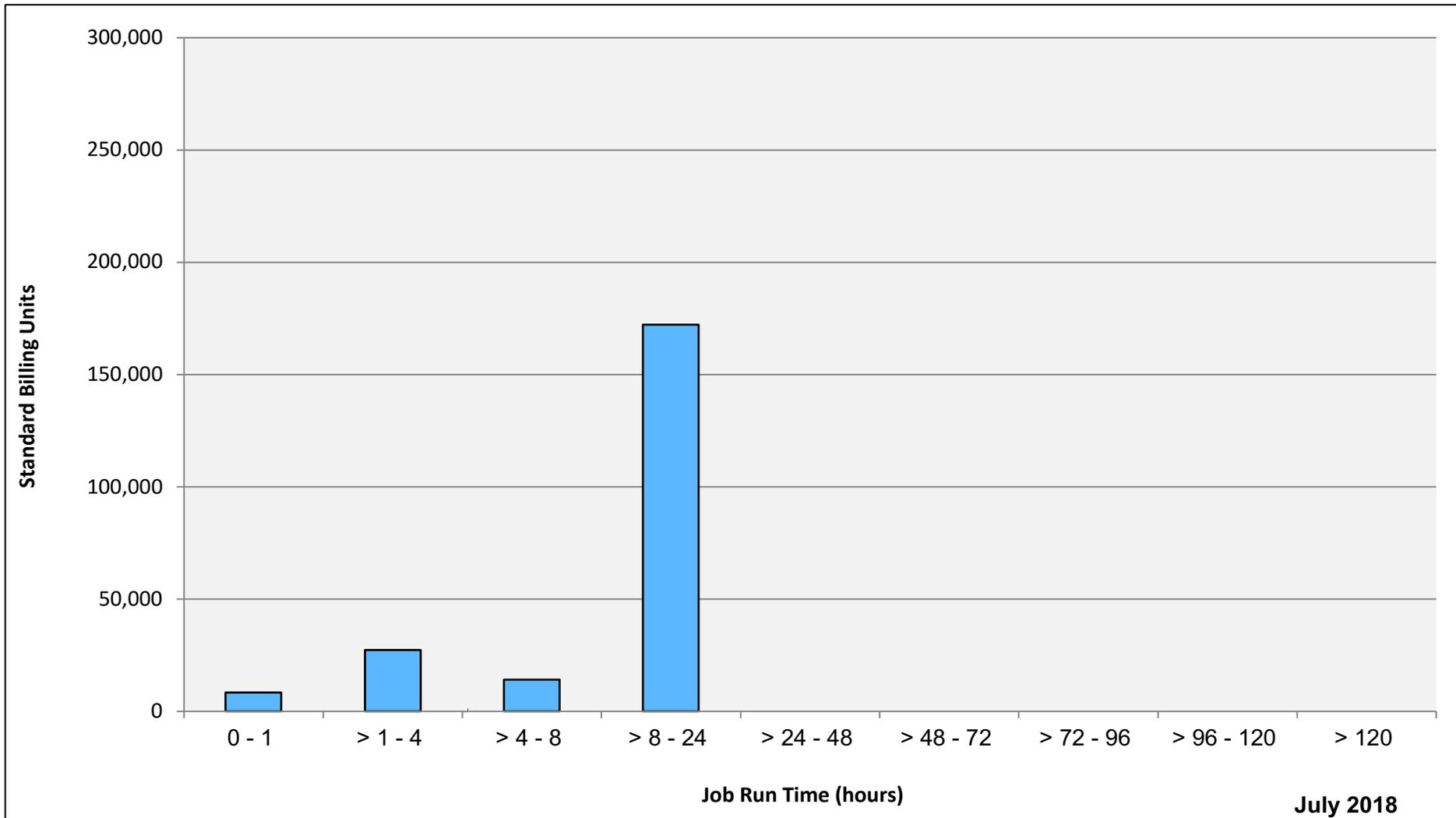
Electra: Average Expansion Factor



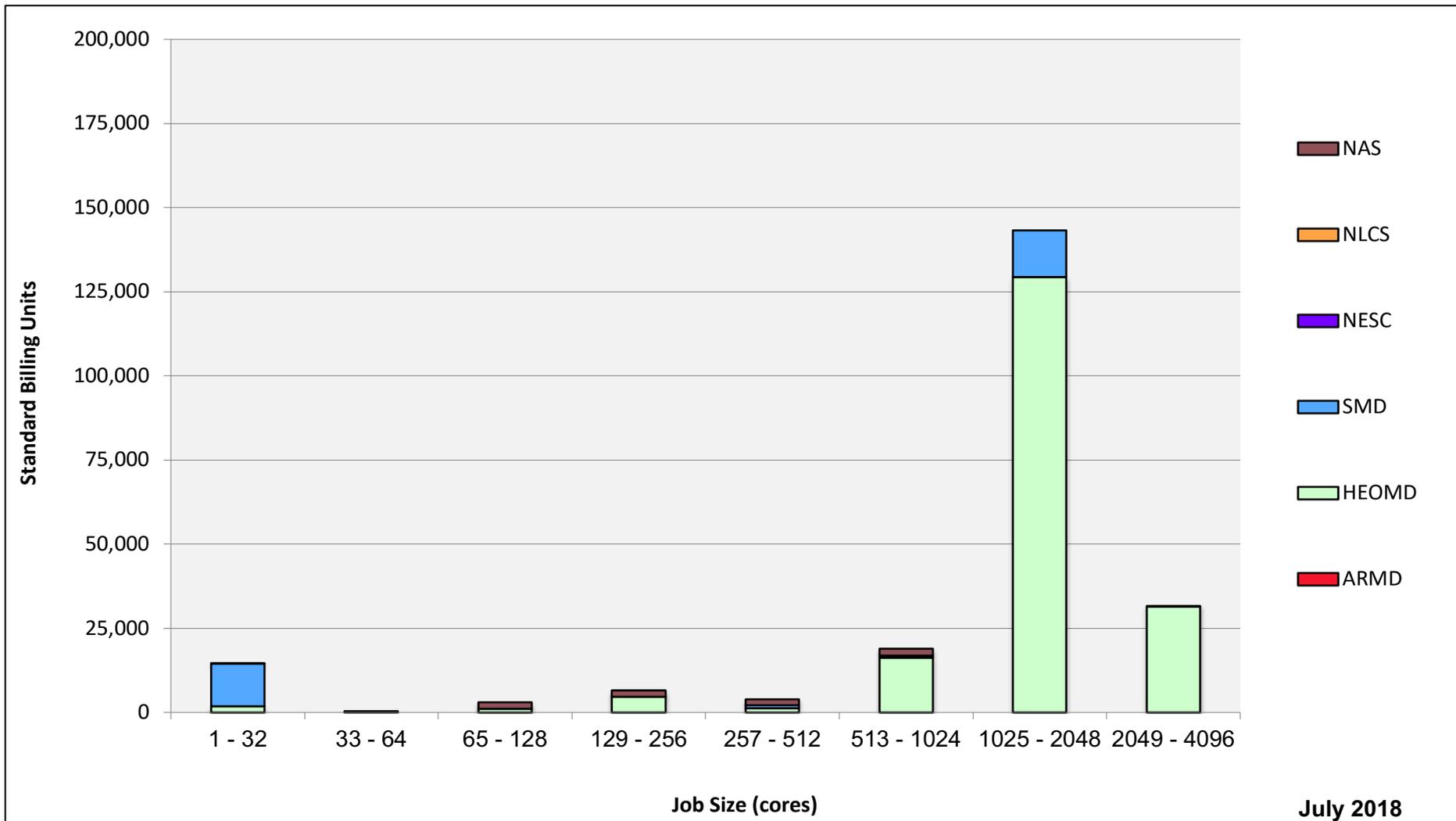
Merope: SBUs Reported, Normalized to 30-Day Month



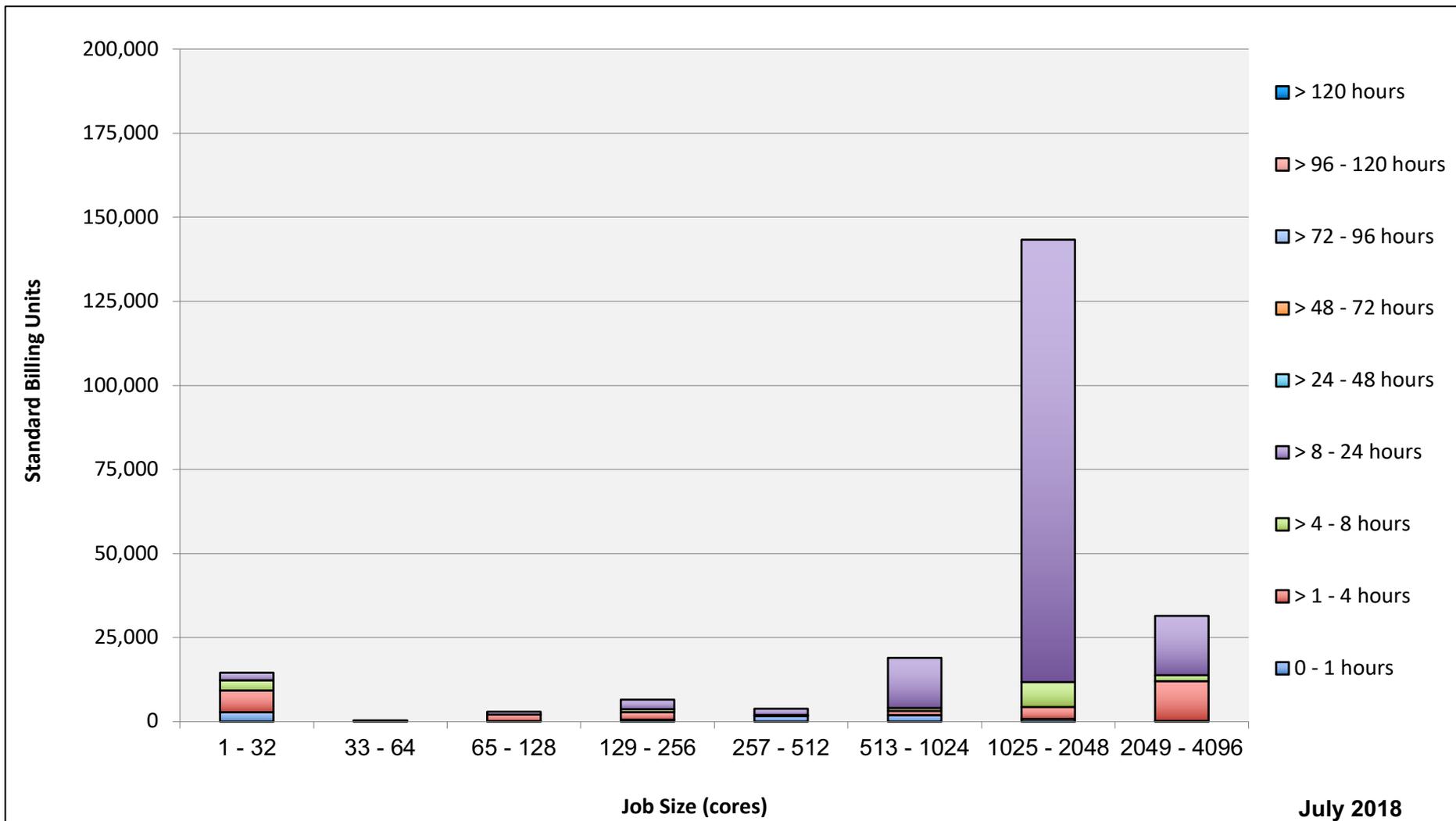
Merope: Monthly Utilization by Job Length



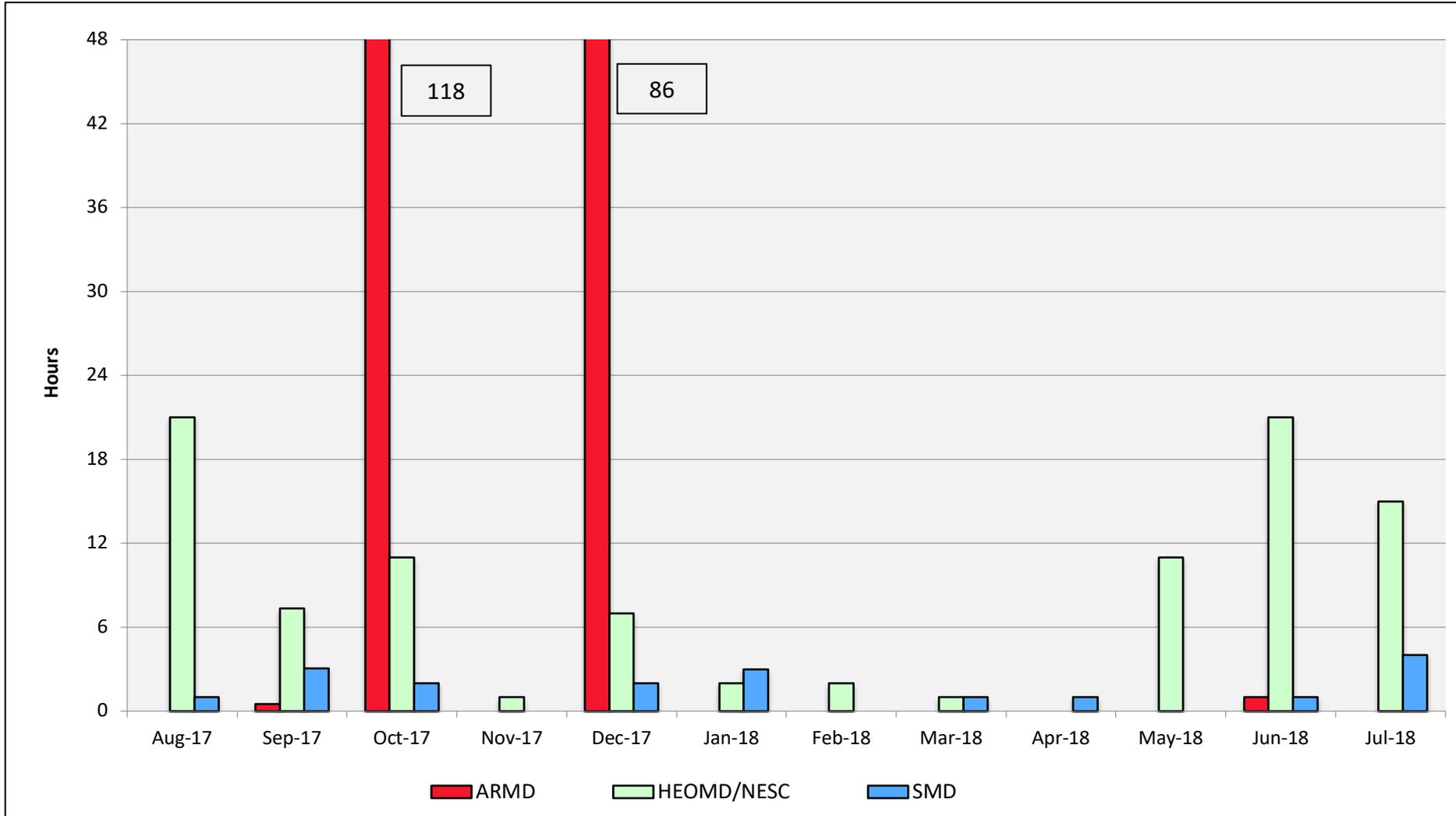
Merope: Monthly Utilization by Size and Mission



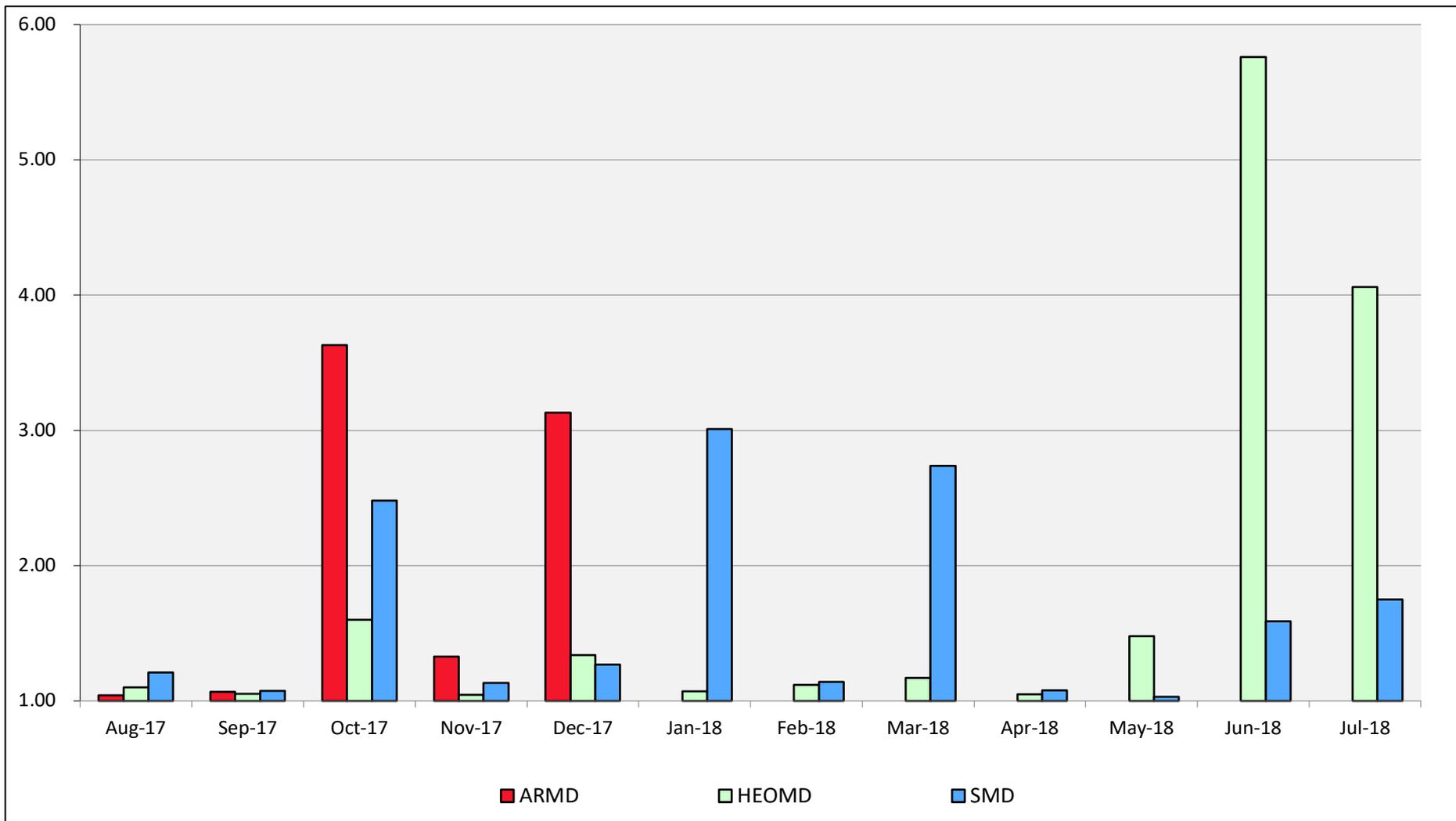
Merope: Monthly Utilization by Size and Length



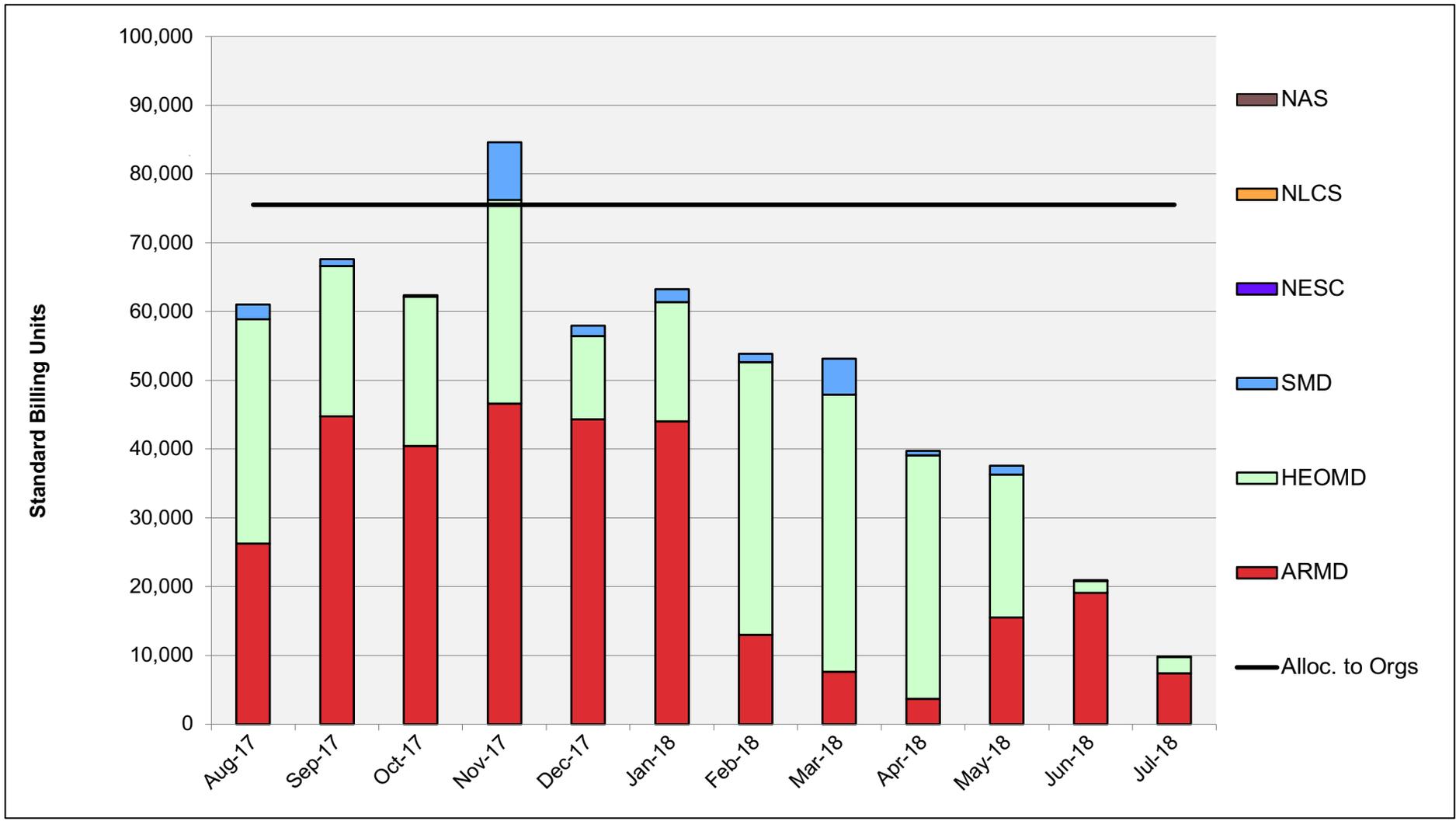
Merope: Average Time to Clear All Jobs



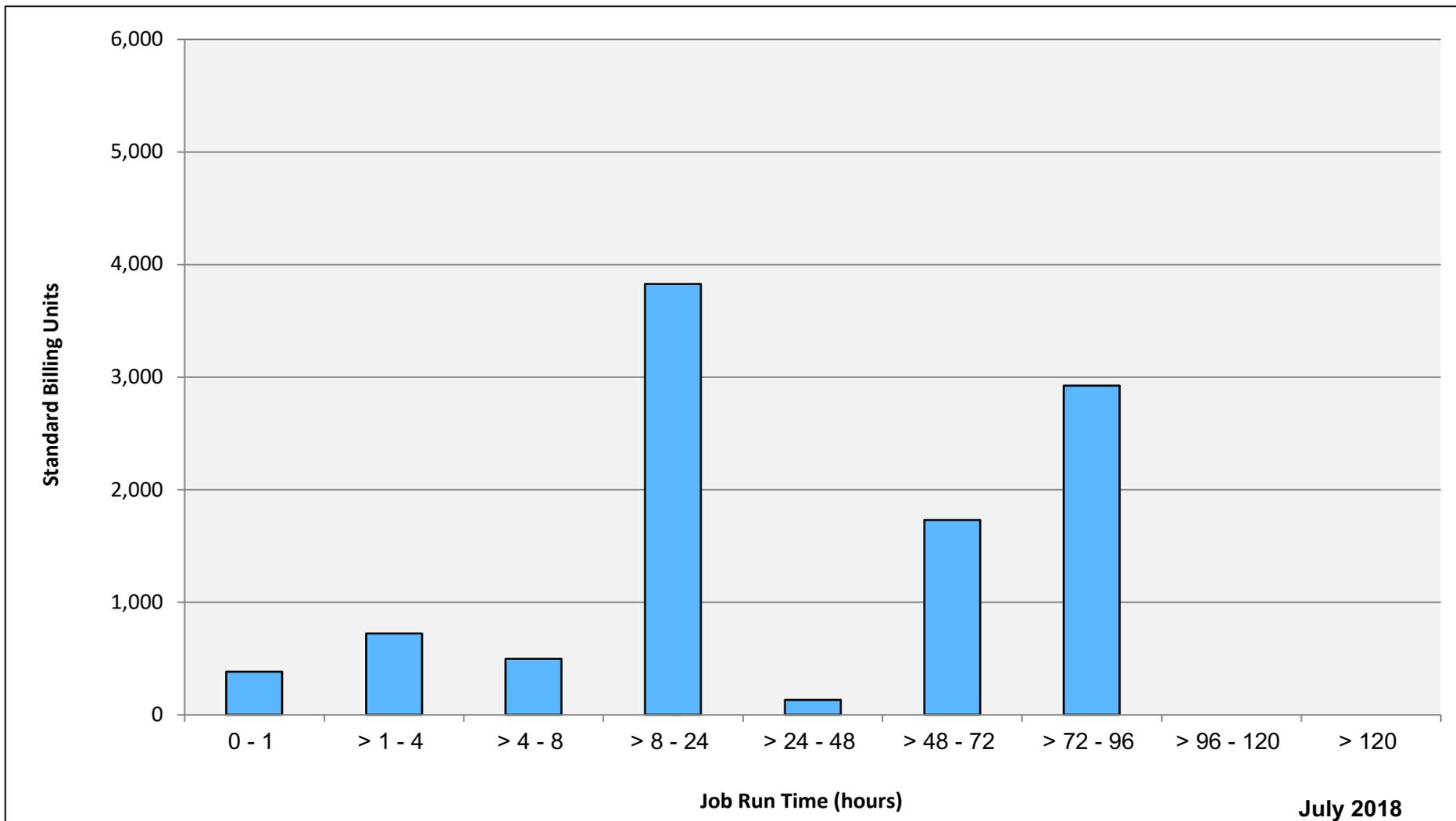
Merope: Average Expansion Factor



Endeavour: SBUs Reported, Normalized to 30-Day Month

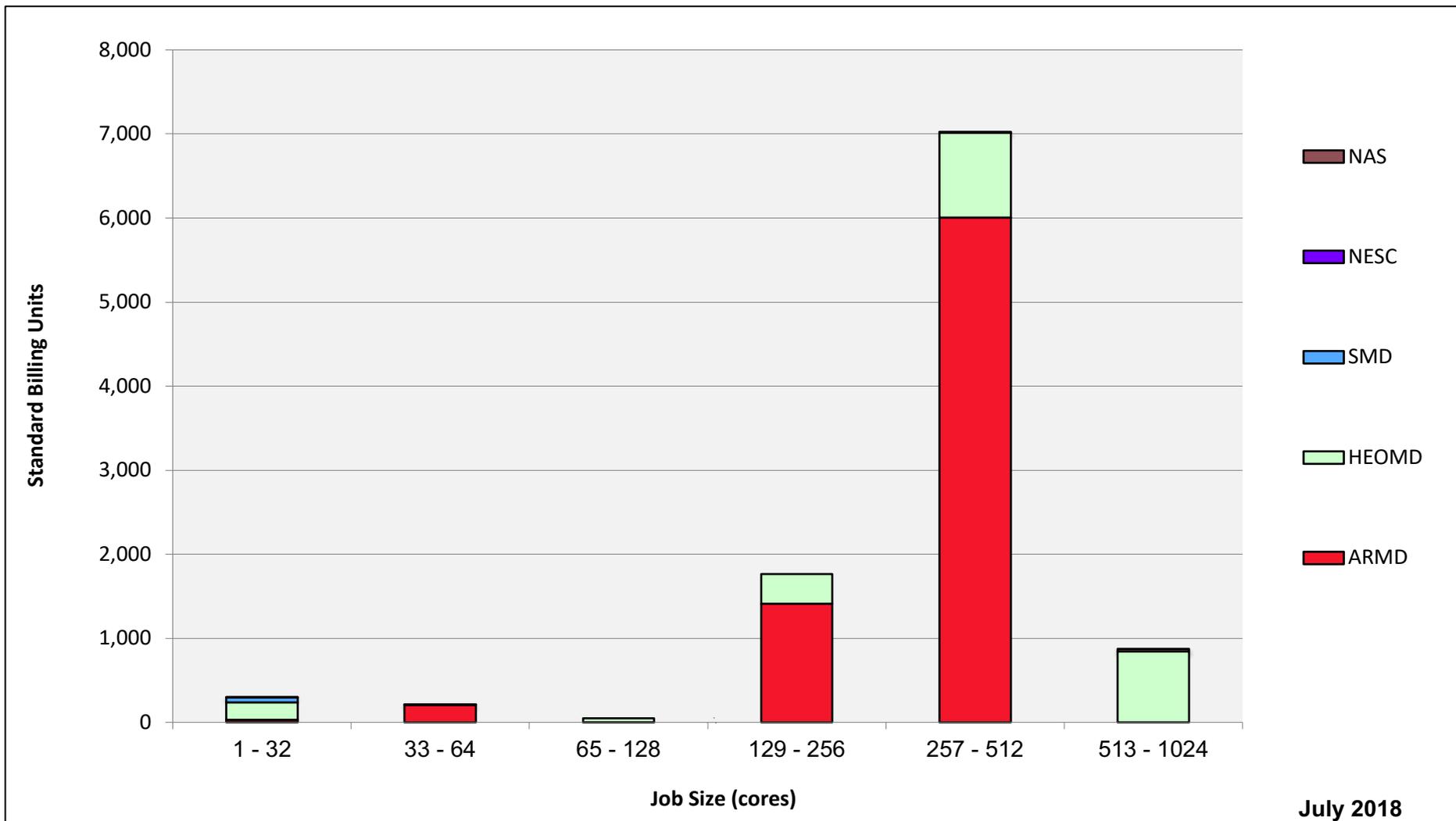


Endeavour: Monthly Utilization by Job Length



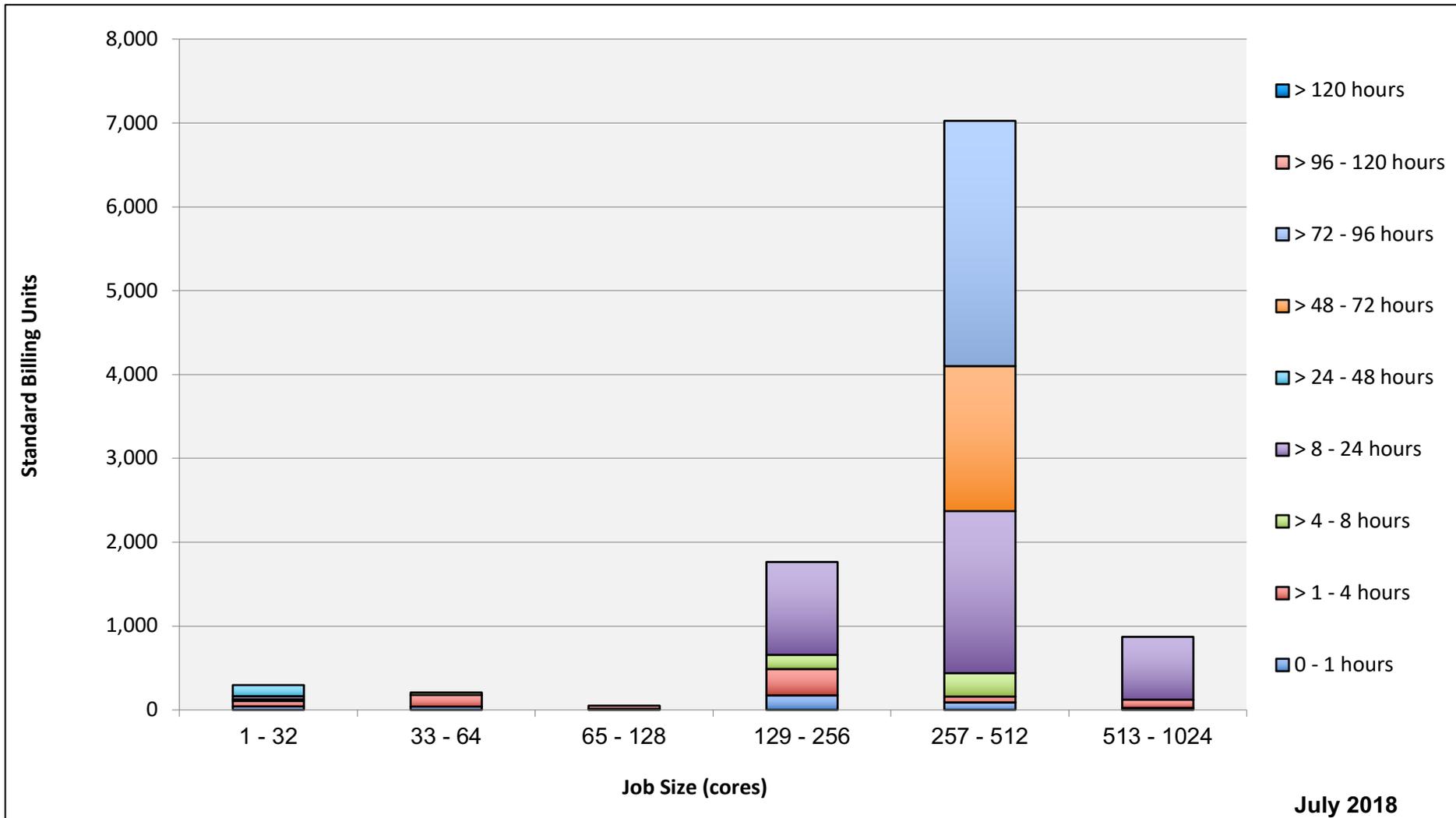
July 2018

Endeavour: Monthly Utilization by Size and Mission



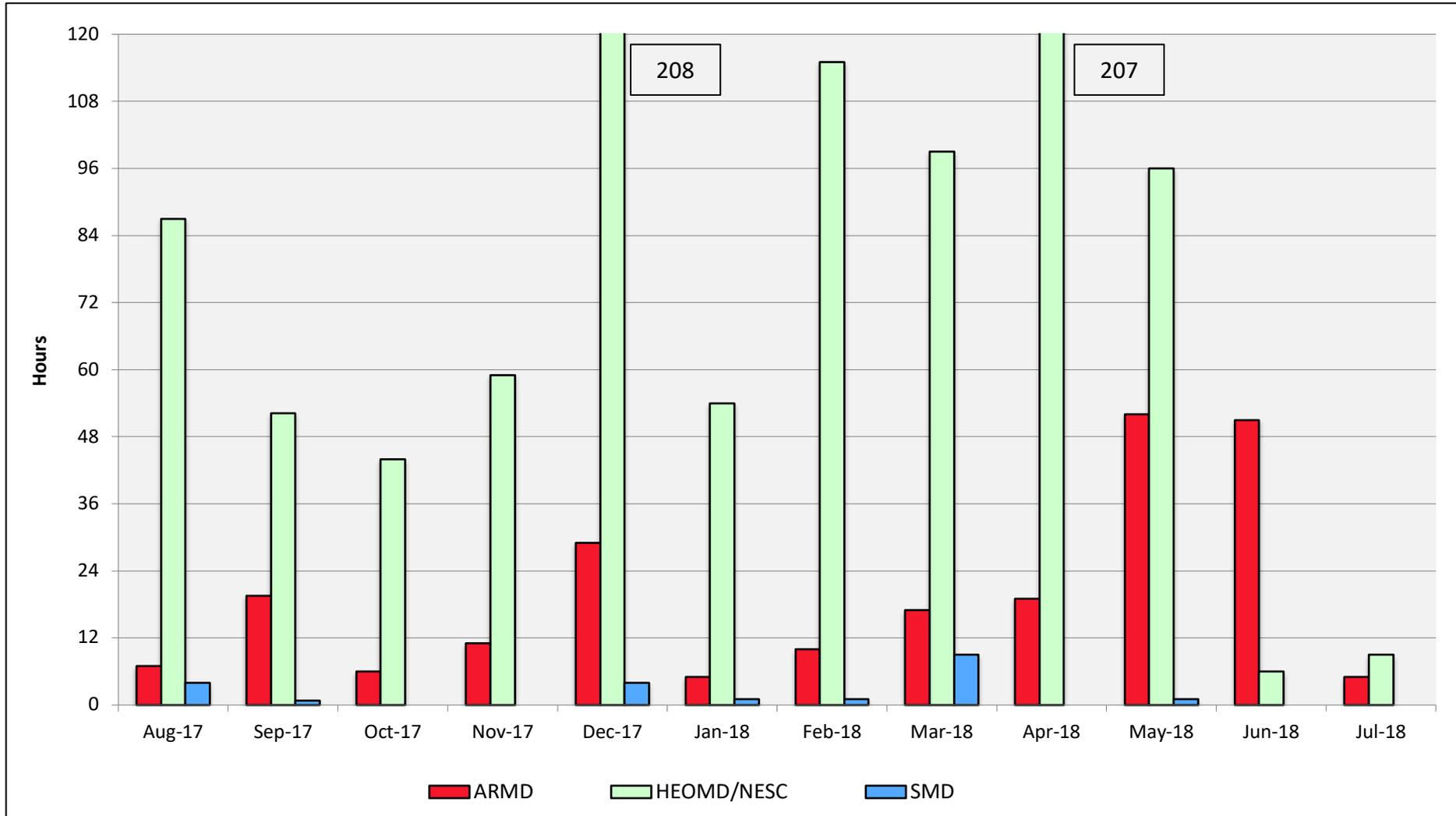
July 2018

Endeavour: Monthly Utilization by Size and Length



July 2018

Endeavour: Average Time to Clear All Jobs



Endeavour: Average Expansion Factor

