

HIGH-END COMPUTING CAPABILITY PORTFOLIO

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NASA Advanced Supercomputing Division

September 10, 2019

HECC Celebrates Grand Opening of New Modular Facility

- HECC and NASA Advanced Supercomputing (NAS) Division staff coordinated and produced the highly successful grand opening of the new Modular Supercomputing Facility, held at NASA Ames on August 22, 2019.
- Ames Center Director Eugene Tu welcomed invited speakers, local and state government officials, the media, and other guests; and spoke about Ames' key role in high-performance computing.
  - Tom Pyke, District Director for Congressman Rho Khanna, representing the 17th District of California, presented a special congressional recognition.
  - NAS Division Chief Piyush Mehrotra served as master of ceremonies.
- Event activities included:
  - Short talks from invited speakers: Tsengdar Lee, HEC Program Manager; Bill Mannel, Vice President and General Manager of High-Performance Computing and Artificial Intelligence, Hewlett Packard Enterprise; and Bill Thigpen, HECC Project Manager.
  - Tours of the new Modular Supercomputing Facility and the new Aitken system.
  - Media question & answer session with Bill Thigpen and scientists who perform modeling and simulation on HECC's modular resources.
  - A festive barbeque lunch for 200-plus guests, hosted and supported by NAS Division volunteers.
- The event was featured by numerous local and tech industry media, including GNC, KQED Public Media, InsideHPC, and others.

IMPACT: The new modular facility will help solve the agency's most challenging problems in an environmentally conscious way that also provides flexibility, power efficiency, and cost savings.

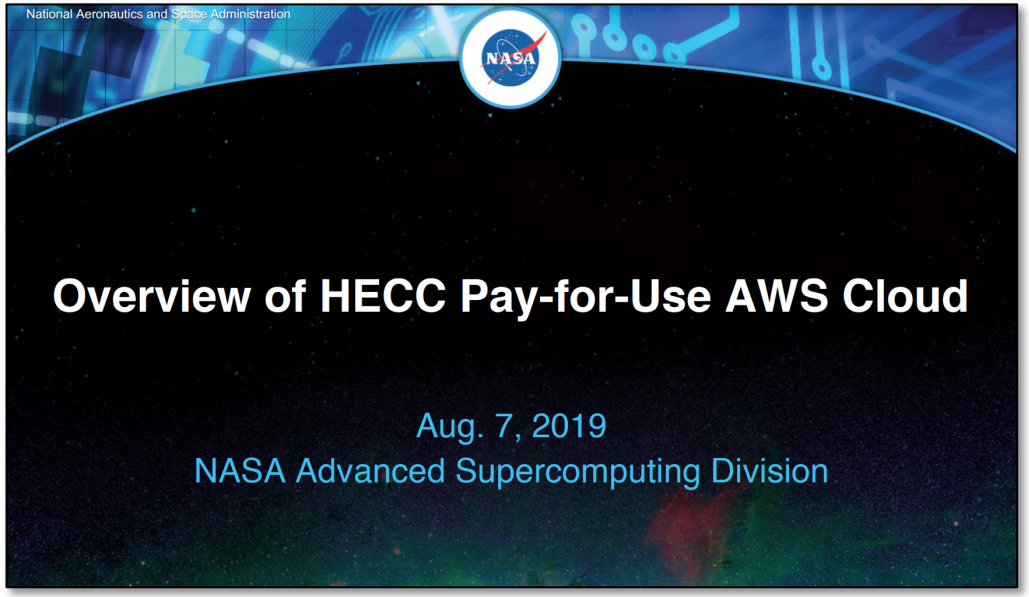


Ribbon-cutting ceremony for the new Modular Supercomputing Facility held at NASA Ames on August 22. *Derek Shaw, NASA/Ames*

Cloud Team Completes Integration of AWS Public Cloud into HECC Production Environment

- On August 7, the Cloud team formally introduced to the HECC user community the Amazon Web Services (AWS) Public Cloud as a logical extension to the production environment.
  - The team conducted a training webinar, which attracted 43 attendees. The slide presentation and recording were made available online afterwards for those who were not able to attend the live event. See: https://www.nas.nasa.gov/hecc/support/past_webinars.html
  - 16 KnowledgeBase articles providing more detailed technical information were published. See: https://www.nas.nasa.gov/hecc/support/kb/175/
- The AWS integration includes the following cost conscious, flexible, and user-friendly implementations:
  - Bursting batch jobs from on-premise PBS server to AWS.
  - Dynamically turning on/off certain AWS resources (front end, PBS servers, filesystems) to save cost.
  - Transferring and/or managing files from either on-premise front ends, AWS front ends, or within PBS job scripts.
  - Viewing Cloud expense records with existing HECC accounting tools.
- Cloud staff are now integrating AWS GovCloud to support projects requiring ITAR and Export Administration Regulations (EAR99).

IMPACT: Offering AWS Cloud provides an alternative to principle investigators who are willing to pay to access state-of-the-art resources not currently available on premise, or to speed up job turnaround time when HECC resources are very busy.

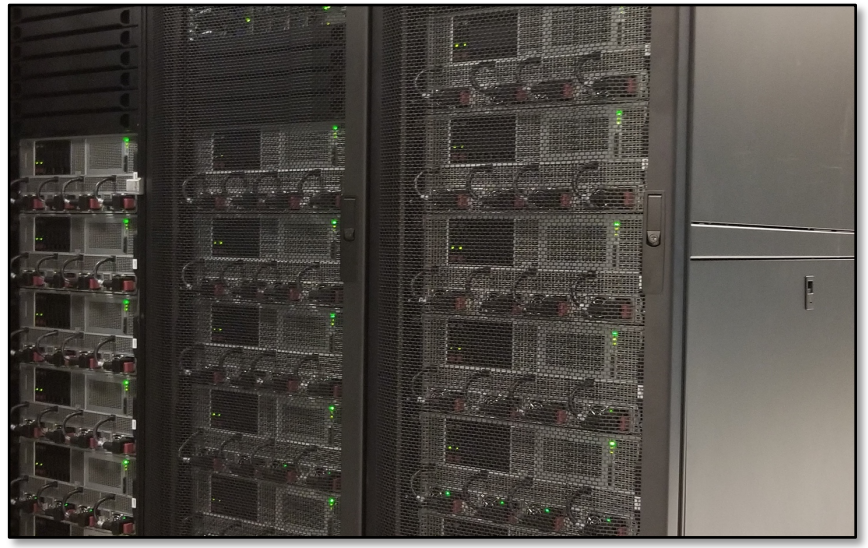


Title page of the August 7, 2019 user training webinar introducing the Pay-for-Use AWS Cloud to the HECC user community.

HECC Holds First GPU Bootcamp After Release to Users

- A highly successful NASA GPU Bootcamp was held August 14–15, 2019.
  - More than 60 people participated in the Bootcamp, split between 30 onsite and 30-plus remote attendees via WebEx.
  - Three hands-on lab sessions and an afternoon mini-code challenge were especially useful to reinforce learning and clarify key concepts. More than 8 teams took part in the mini-code challenge and attained speed-ups ranging from 4–15 times over the initial CPU-only code.
  - NVIDIA staff provided the training, which was very well received, and several attendees requested copies of the training material.
- The V100 GPU nodes were released into production on June 21.
  - More than 20 users and HECC staff have run jobs on these nodes.
  - The jobs have been a mixture of 64% machine learning/deep learning (ML/DL) and 36% HPC applications, in terms of SBU usage.
  - The dominant ML/DL application uses python with the PyTorch deep learning framework to perform a temporal interpolation between two consecutive snapshots of GOES-16 ABI data. A single V100 GPU card provides a factor of 8 speed-up over the older K40 GPUs.
  - The dominant HPC application used on the GPUs is FUN3D, a CFD suite of codes and tools developed at NASA Langley.

IMPACT: The GPU Bootcamp provided an easy introduction to GPU programming and unleashed an unprecedented wave of interest from the HECC user community. Existing python ML/DL frameworks enable Earth Science users to quickly take advantage of the performance boost provided by the V100 GPUs over the older K40 GPUs.

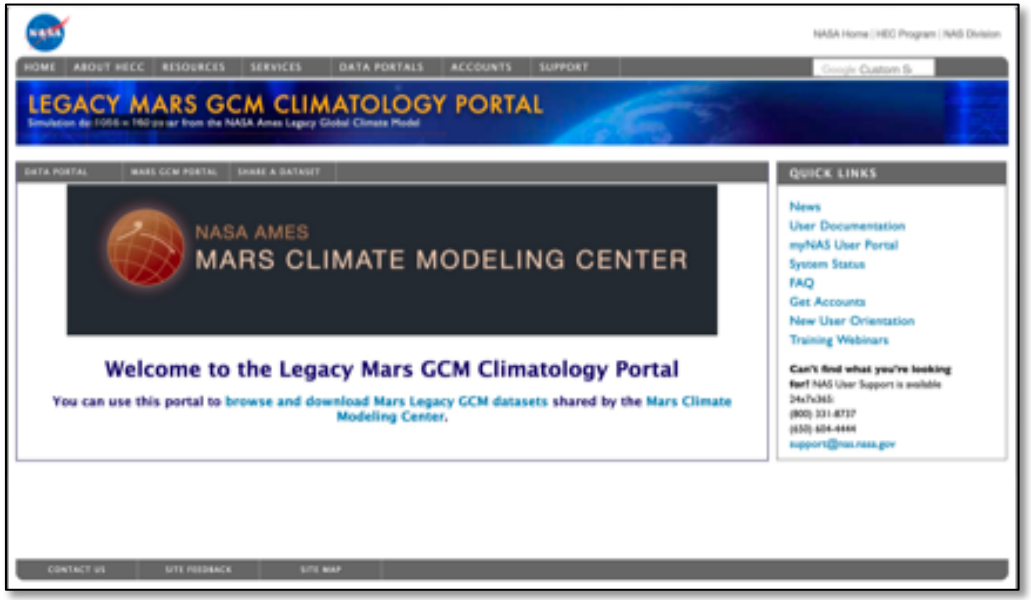


HECC's new NVIDIA GPU unit nodes are housed in three racks on the NASA Advanced Supercomputing facility's main computer floor. *Johnny Chang, NASA/Ames*

Mars GCM Dataset Shared Through HECC Data Portal

- HECC's Big Data and Analytics team worked with the Mars Climate Modeling Center to add the Legacy Mars General Circulation Model (GCM) Climatology dataset to the HECC Data Portal. The dataset:
  - Includes 19 gigabytes (GB) in 71 files of data for one Mars year from the NASA Ames Legacy GCM.
  - Comprises simulations of observed water cycle to determine water sources and sinks.
  - Simulations include enhanced interactions of dust, carbon dioxide, and water cycles.
- The team also made enhancements to the HECC Data Portal to improve future scalability.
  - Functional upgrades to improve file loading for datasets with many files.
  - Pagination function to load dataset files in selectable sets of a thousand.
  - File statistics are stored in the database, to avoid frequent filesystem traversal.
- The original data portal pages were restyled to blend with the look of the HECC website.

IMPACT: The HECC Data Portal is leveraged to share large datasets from Mars climate simulations. The Data Portal provides researchers with a platform to share large datasets with collaborators or the public to promote innovation and scientific discovery.



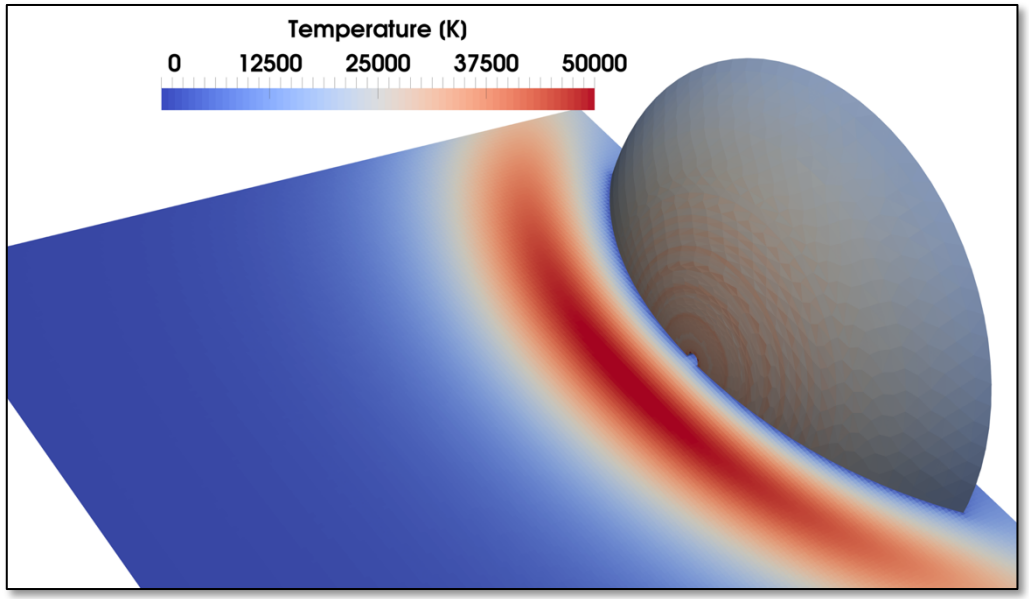
The landing page of the new Mars GCM data portal serves as the entryway to the downloadable dataset files.

Hypervelocity Sampling of Venus' Noble Gases*

- Researchers from NASA's Ames Research Center and Jet Propulsion Laboratory used the Pleiades supercomputer to perform 2D axisymmetric and full 3D direct simulation Monte Carlo (DSMC) simulations of the Cupid's Arrow probe with the SPARTA software package.
- Cupid's Arrow is a small satellite probe mission concept that would determine the amount of noble gases and associated isotope ratios in Venus' atmosphere.
- Performing high-fidelity noble gas measurements in Venus' atmosphere can help explain why Earth and Venus have diverged in their geological evolution—a critical piece of information scientists need to better assess whether a terrestrial exoplanet is Earth-like or Venus-like.
- Preliminary simulations on a simplified spacecraft and sampling system in both 2D and 3D configurations show that while there is no significant isotopic fraction for xenon or argon isotopes, the total ratio of argon to xenon does change throughout the domain.
- The team used the SPARTA DSMC code to run their simulations in parallel, with one simulation using up to 2,048 processors during 72 hours for the 3D simulations.

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

IMPACT: Simulations performed in order to investigate the sensitivity of the numerical results to a wide range of parameters, will help inform the overall spacecraft and sampling system design.



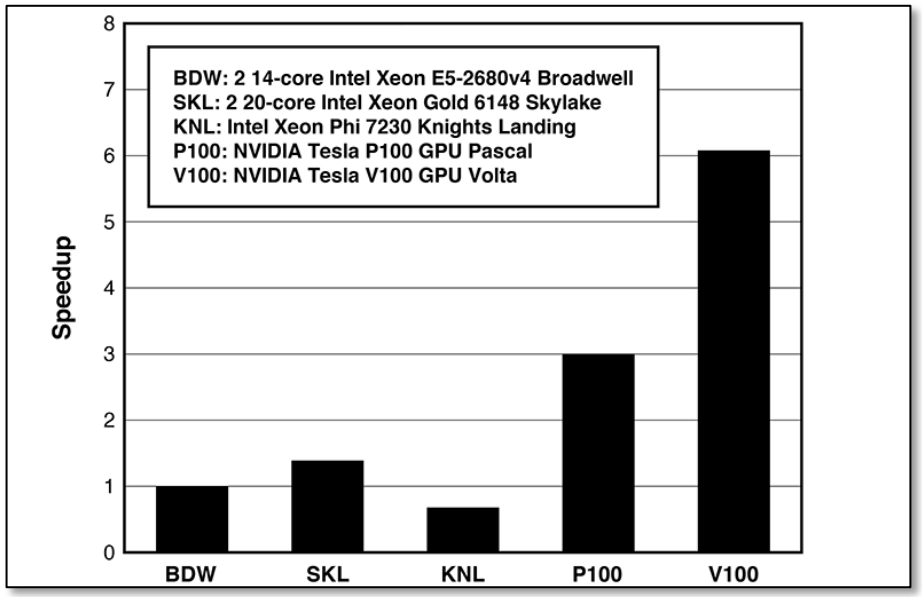
Visualization of the surface of the Cupid's Arrow concept satellite, with a view of the flow and bow shock in front of the spacecraft. Red to blue in the 2D slice represents hot (50,000 K) to cold (0 K). Red to blue on the heat shield represents high to low heat flux. *Michail Gallis, Sandia National Laboratories, Arnaud Borner, NASA/Ames*

Preparing the FUN3D Solver for the Exascale Era*

- Researchers at NASA Langley studied next-generation computational performance for the NASA unstructured-grid Navier-Stokes flow solver FUN3D. The team explored a wide range of programming models appropriate for the many-core architectures driving the current landscape of leadership-class HPC facilities.
  - The work was part of a multi-year effort done in collaboration with industry, university, and government partners.
  - The team used mini-applications to investigate several programming models, and ultimately chose a CUDA-based approach to port and optimize the complete suite of FUN3D kernels required to solve the Navier-Stokes equations; the entire solution is computed on GPUs with minimal data transfer between CPUs and GPUs.
- Pleiades and Electra were used extensively for node-level, Intel Xeon-based optimization and profiling exercises. The study showed:
  - A single NVIDIA Tesla V100 GPU delivers a computational speedup of about 4.3 times that of a heavily optimized code running on a dual-socket Intel Xeon Gold 6148 Skylake processor containing 40 cores.
  - Tests showed a nominal 30 times speedup advantage for the GPU approach—or a total throughput equivalent to that of about a million CPU cores.
- The Langley researchers acknowledged hardware experts at the NASA Advanced Supercomputing facility for critcal reviews that were “invaluable to the effort.”

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

IMPACT: With this approach to optimizing NASA’s FUN3D flow solver, a thousand of today’s 6-GPU nodes can do the work of over a million CPU cores for a fraction of the energy cost.



Performance of an unsteady Navier-Stokes simulation on common high-performance computing architectures is shown relative to a dual-socket node with two Intel Xeon E5-2680v4 Broadwell processors. *Aaron Walden, Eric Nielsen, NASA/Langley*

User Outreach Tour Aims to Improve Productivity

- In August, a contingent of HECC staff visited users at Glenn Research Center to highlight the project's extensive resources and services.
- The team held a successful discussion session with more than 20 scientists, engineers, and partners who depend on HECC resources and services for their NASA missions.
  - Users had the opportunity to ask questions and receive detailed information about the full range of services available to improve efficiency on HECC systems.
  - There was strong interest in how to request new software and get additional help from applications experts for very new users to plan code architecture.
  - Users were also interested in getting allocations for more compute resources and reservations to do more leading edge research.
- The team will go to Johnson Space Center in September and 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.

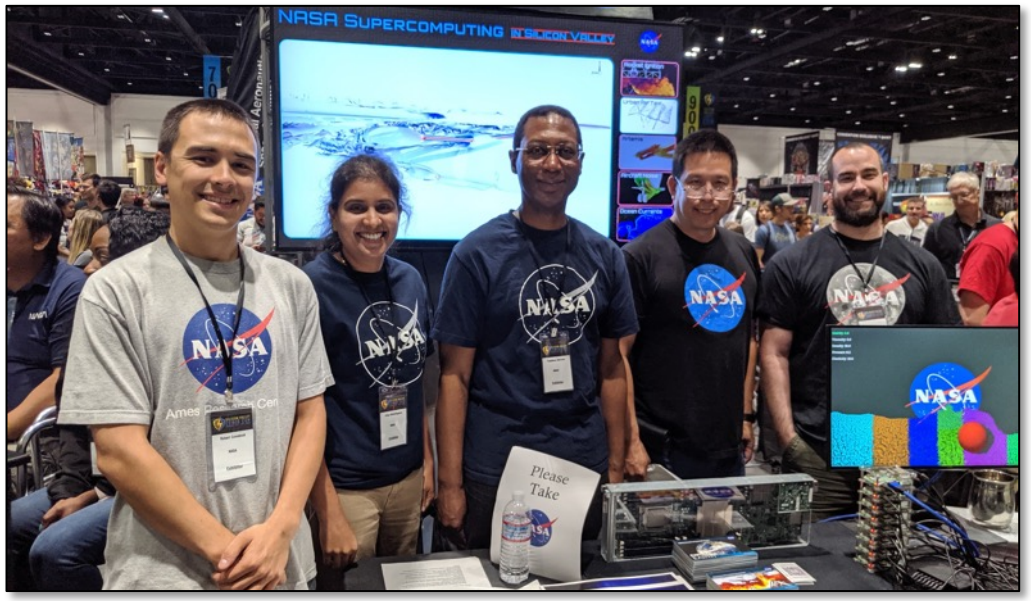


Image of Glenn Research Center. *Jennifer Rock, NASA*

HECC Supercomputing Shines at Silicon Valley Comic Con

- For the third year, a team of HECC researchers and support staff produced an outstanding outreach exhibit in the NASA booth at Silicon Valley Comic Con (SVCC), held August 16–18, 2019, in San Jose, CA. Attendance was estimated at 70,000.
  - The exhibit was part of an extensive NASA presence, which included a full-scale model of the Mars Curiosity Rover, three NASA-specific panels, and a guest appearance by ISS Commander Chris Hadfield.
  - HECC staff greeted thousands who were eager to speak with experts about the role of supercomputing in the agency's projects and missions.
- The HECC video jukebox tool was updated with new visualizations, titles, and captions, including: Urban air mobility, ocean circulation modeling, aircraft landing gear noise, and Artemis booster separation and launch environment.
- This year's exhibit included our Raspberry Pi cluster demo, which explains distributed computing in an interactive, easy-to-understand way; instructions for building a similar cluster were also provided.
- HECC users Marie Denison and Sarah D'Souza were featured on SVCC's Women of NASA Panel, and described the types of data they compute and simulations they run on HECC resources.

IMPACT: NASA's exhibit at SVCC each year provides an excellent public outreach opportunity to highlight the critical role of HECC resources in science and engineering across the agency.



The HECC exhibit attracted thousands at SVCC, including Ames Research Center Director Eugene Tu (second from right). Also pictured (l-r): Robert Comstock, Vidya Bobbligama, Thaddeus Norman, and Michael Hartman. *Blaise Hartman, NASA/Ames*

HECC Facility Tours in August 2019

- HECC hosted 19 tour groups in August; 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:
  - Thomas Zurbuchen, NASA Associate Administrator.
  - Sandra Cauffman, NASA Acting Director for the Earth Science Division.
  - Steve Jurczyk, NASA Associate Administrator and Melanie Saunder, Deputy Associate Administrator.
  - Renee Wynn and Jeff Seaton, NASA Chief Information Officers.
  - U.S. Congressman Brian Babin, serving the 36th District of Texas.
  - Giorgio Saccoccia, President of the Italian Space Agency (ASI).
  - Attendees of the ASME-JSME-KSME (American Society of Mechanical Engineers-Japan Society of Mechanical Engineers-Korean Society of Mechanical Engineers) Joint Fluids Engineering Conference, held in San Francisco.
  - NASA Continuous Mitigation and Diagnostics group from Kennedy Space Center.



Ames Center Director Eugene Tu (second from right) and NAS Division Chief Piyush Mehrotra (far left) discuss the Estimating the Circulation and Climate of the Ocean (ECCO) model with Congressman Brian Babin. NAS Visualization team lead Chris Henze (standing), shows the ECCO global ocean simulations on the hyperwall.

Papers

- "**Simulation of the 2019 Global Dust Storm on Mars Using the NASA Ames Mars GCM: A Multi-Tracer Approach**," T. Bertrand, et al., arXiv:1908.02453 [astro-ph.EP], August 7, 2019. * https://arxiv.org/abs/1908.02453
- "**Numerical Investigation of the Effect of Obstacle Shape on Deflagration to Detonation Transition in a Hydrogen-Air Mixture**," A. Coats, D. Mathias, B. Cantwell, Combustions and Flame (Elsevier), vol. 209, published online August 13, 2019. * https://www.sciencedirect.com/science/article/pii/S0010218019303542
- "**Pickup Ions Beyond the Heliopause**," V. Roytersheteyn, N. Pogorelov, J. Heerikhuisen, The Astrophysical Journal, vol. 881, no. 1, August 13, 2019. * https://iopscience.iop.org/article/10.3847/1538-4357/ab2ad4/meta
- "**The Formation of Ultra-Diffuse Galaxies from Passive Evolution in the RomulusC Galaxy Cluster Simulation**," M. Tremmel, et al., arXiv:1908.05684 [astro-ph.GA], August 15, 2019. * https://arxiv.org/abs/1908.05684
- "**Numerical Investigation and Optimization of a Flushwall Injector for Scramjet Applications at Hypervelocity Flow Conditions**," T. Drozda, et al., presented at the AIAA Propulsion and Energy 2019 Forum, Indianapolis, IN, August 19-22, 2019. * https://arc.aiaa.org/doi/abs/10.2514/6.2019-4196

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

Papers (cont.)

- "**Quantification of Surface Forcing Requirements for a Greenland Ice Sheet Model Using Uncertainty Analyses**," N.-J. Schlegel, E. Larour, Geophysical Research Letters (early view), August 19, 2019. * https://agupubs.onlinelibrary.wiley.com/doi/full/10.1029/2019GL08353
- "**A Brief Review on Particle Acceleration in Multi-Island Magnetic Reconnection**," H. Che, G. Zank, arXiv:1908.09155 [astro-ph.SR], August 24, 2019. * https://arxiv.org/abs/1908.09155
- "**Impacts of Dust-Radiation Versus Dust-Cloud Interactions on the Development of a Modeled Mesoscale Convective System over North Africa**," C.-C. Huang, et al., Monthly Weather Review, August 26, 2019. * https://journals.ametsoc.org/doi/full/10.1175/MWR-D-18-0459.1
- "**Unfolding Overlapped Slitless Imaging Spectrometer Data for Extended Sources**," A. Winebarger, et al., The Astrophysical Journal, vol. 882, no. 1, published online August 27, 2019. * https://iopscience.iop.org/article/10.3847/1538-4357/ab21db

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

News and Events

- **New Modular Supercomputing Facility Opens at NASA's Ames Research Center**, *NAS News Item*, August 19, 2019-- The energy-efficient facility houses NASA's newest supercomputer, named Aitken, to help solve the agency's most challenging science and engineering problems.
  https://www.nas.nasa.gov/publications/news/2019/08-22-19.html
- **Coverage of the Grand Opening of the new Modular Supercomputing Facility and Aitken System**:
  - **NASA Invites Media to the Grand Opening of Modular Supercomputing Facility**, *NASA Ames Media Alert*, August 19, 2019. https://www.nasa.gov/press-release/ames/nasa-invites-media-to-the-grand-opening-of-modular-supercomputing-facility
  - **NASA Celebrates the Grand Opening of Its New Modular Supercomputing Facility**, *NASA Ames Feature*, August 23, 2019. https://www.nasa.gov/image-feature/ames/nasa-celebrates-the-grand-opening-of-its-new-modular-supercomputing-facility
  - **Aitken Supercomputer Will Simulate NASA Moon Landings**, *PC Magazine*, August 26, 2019. https://www.pcmag.com/news/370388/aitken-supercomputer-will-simulate-nasa-moon-landings
  - **NASA Ames' computer powerhouse gets a major upgrade**, *Mountain View Voice*, August 26, 2019. https://mv-voice.com/news/2019/08/26/nasa-ames-computer-powerhouse-gets-a-major-upgrade
  - **NASA's new HPE-built supercomputer will prepare for landing Artemis astronauts on the Moon**, *TechCrunch*, August 22, 2019. https://techcrunch.com/2019/08/22/nasas-new-hpe-built-supercomputer-will-prepare-for-landing-artemis-astronauts-on-the-moon/
  - **HPE Builds NASA New Supercomputer to Support Future Human Mission to Moon**, *Business Wire*, August 22, 2019. https://www.businesswire.com/news/home/20190822005719/en/
  - **NASA's new moon-landing supercomputer is more powerful and more eco-friendly**, *Engadget*, August 26, 2019. https://www.engadget.com/2019/08/26/nasa-eco-friendly-supercomputer/

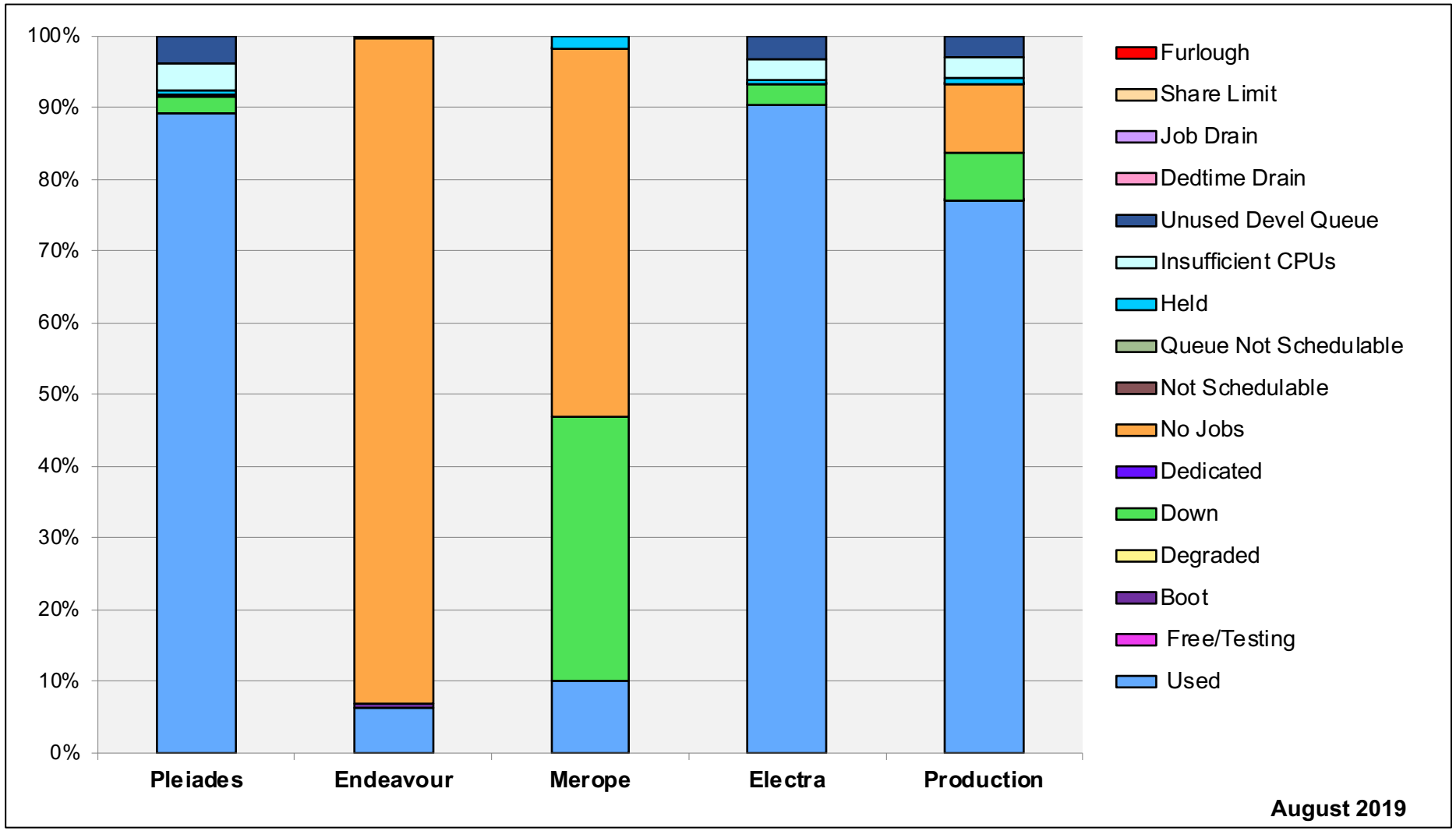
News and Events (cont.)

- **Coverage of the Grand Opening of the new Modular Supercomputing Facility and Aitken System (cont.):**
  - **Scientists Thrill as NASA Ames Launches Supercomputing Facility**, *KQED News*, August 24, 2019. https://www.kqed.org/news/11769784/scientists-thrill-as-nasa-ames-launches-supercomputing-facility
  - **Aitken Supercomputer from HPE to Support NASA Moon Missions**, *insideHPC*, August 22, 2019. https://insidehpc.com/2019/08/aitken-supercomputer-from-hpe-to-support-nasa-moon-missions/
  - **HPE Builds NASA New Supercomputer to Support Future Human Mission to Moon**, *HPCwire*, August 22, 2019. https://www.hpcwire.com/off-the-wire/hpe-builds-nasa-new-supercomputer-to-support-future-human-mission-to-moon/
  - **HPE builds NASA new supercomputer to support future human mission to moon**, *Hewlett Packard Enterprise*, August 22, 2019. https://www.hpe.com/us/en/newsroom/press-release/2019/08/hpe-builds-nasa-new-supercomputer-to-support-future-human-mission-to-moon.html

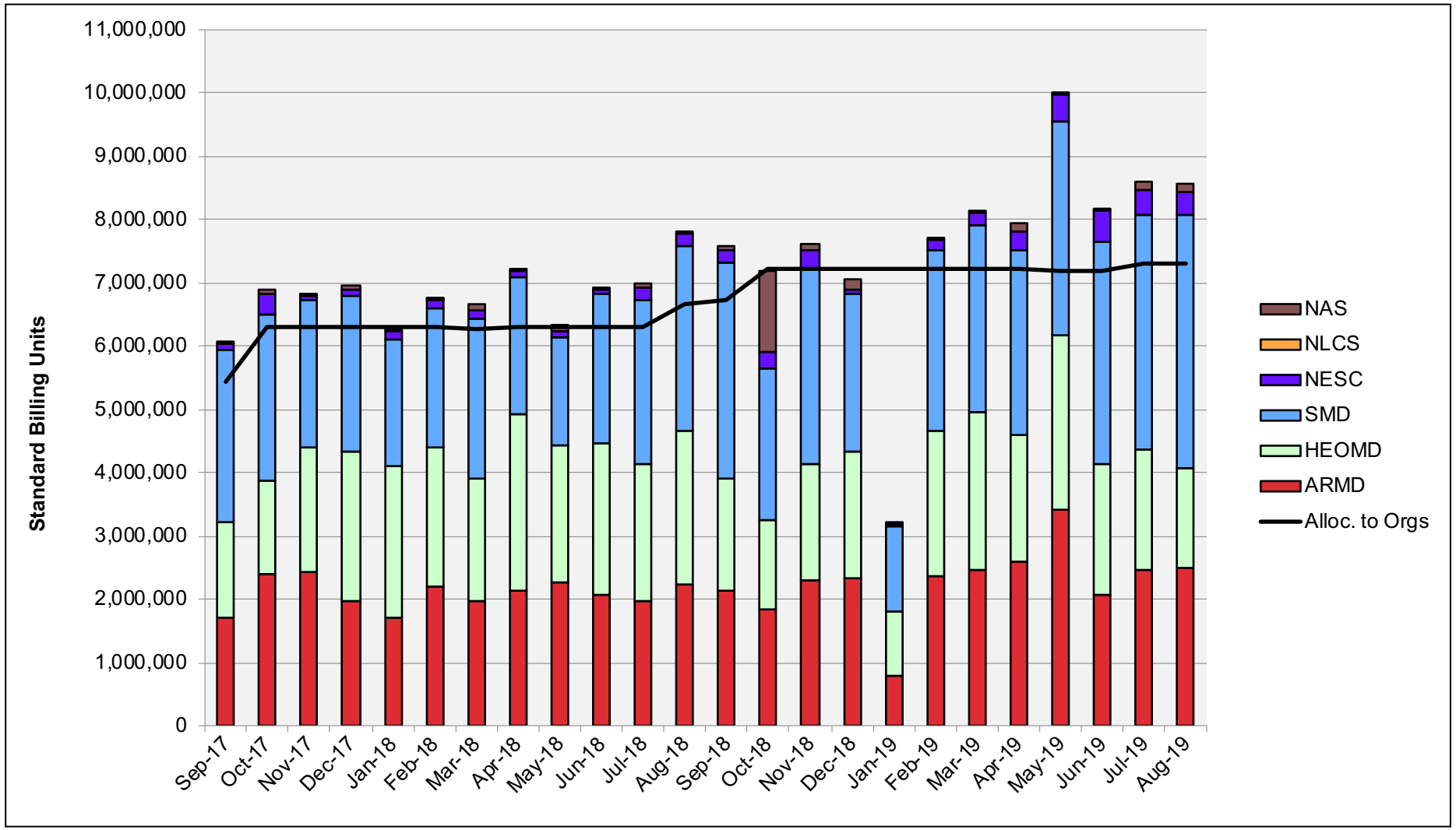
News and Events: Social Media

- **Media Coverage of Modular Supercomputing Facility/Aitken System Opening:**
  - Twitter: NASA Ames, TechCrunch, insideHPC, HPCwire, KQED Science, KQED, Engadget
  - Facebook: NASA Ames, PCMag, Engadget
  - YouTube: Engadget
  - Instagram: NASA Ames
- **Coverage of Silicon Valley Comic Con**
  - NASA Exhibit Twitter: 10 retweets, 12 likes
  - NAS Twitter: 2 retweets, 4 likes; Twitter: 1 retweet; Twitter: 6 retweets, 12 likes
- **Top Posts from NAS**
  - Modular Supercomputing Facility/Aitken
    - Facebook: 531 users reached, 30 engagements
    - Twitter: 7 retweets, 10 likes; Twitter: 9 retweets, 16 likes
  - NASA Spinoff – Computational Fluid Dynamics for Aeronautics
    - Facebook: 387 users reached, 13 engagements
    - Twitter: 4 likes; Twitter: 2 retweet, 6 likes

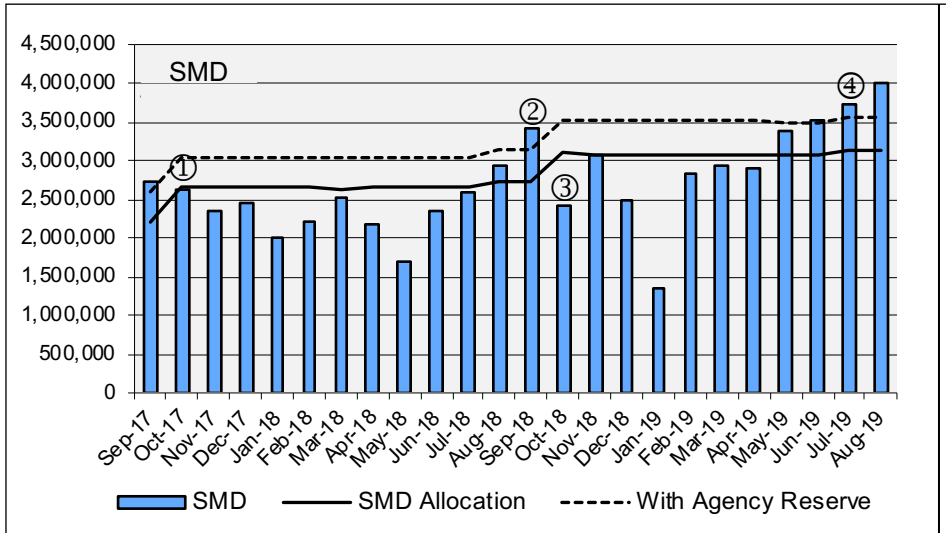
HECC Utilization

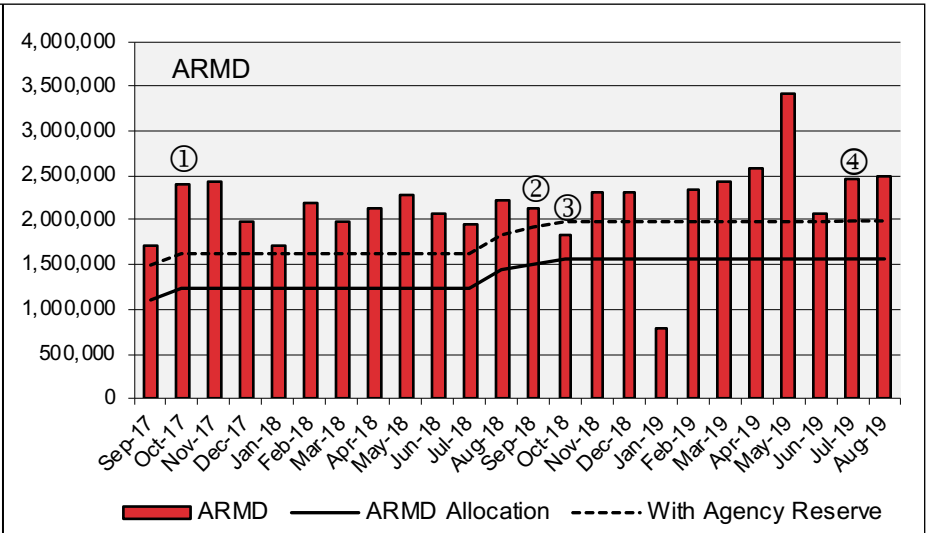


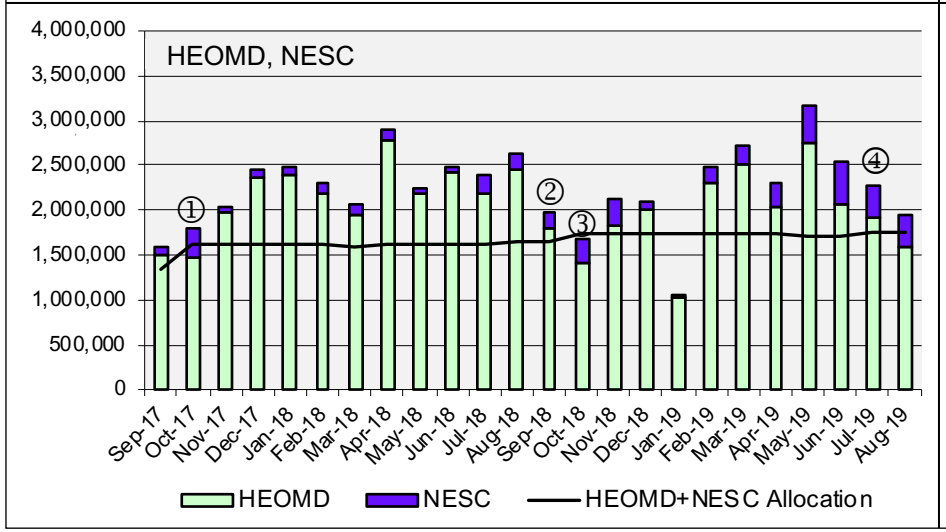
HECC Utilization Normalized to 30-Day Month



HECC Utilization Normalized to 30-Day Month







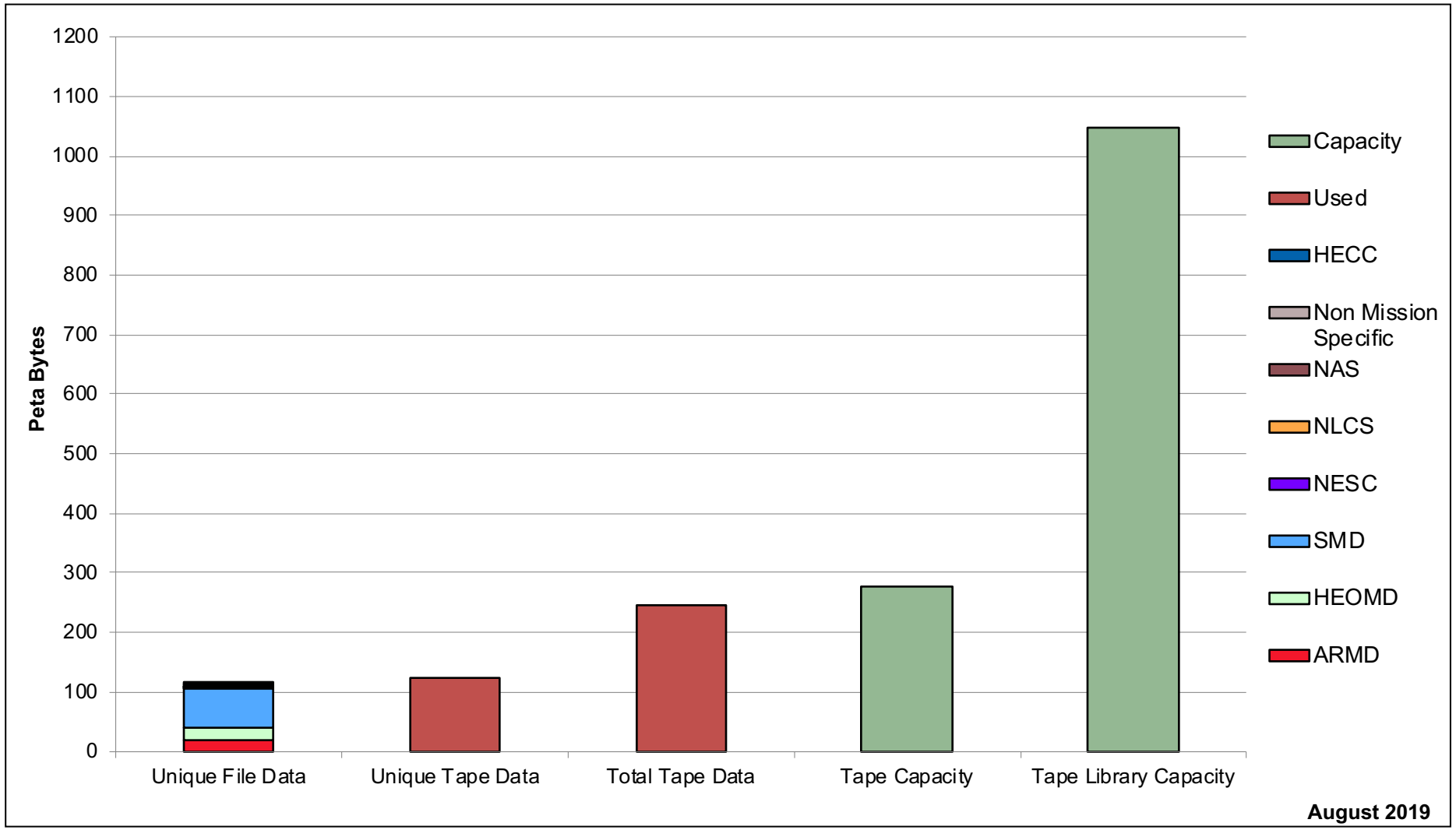
① 4 Skylake E cells (16 D Rack Equivalence) added to Electra

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

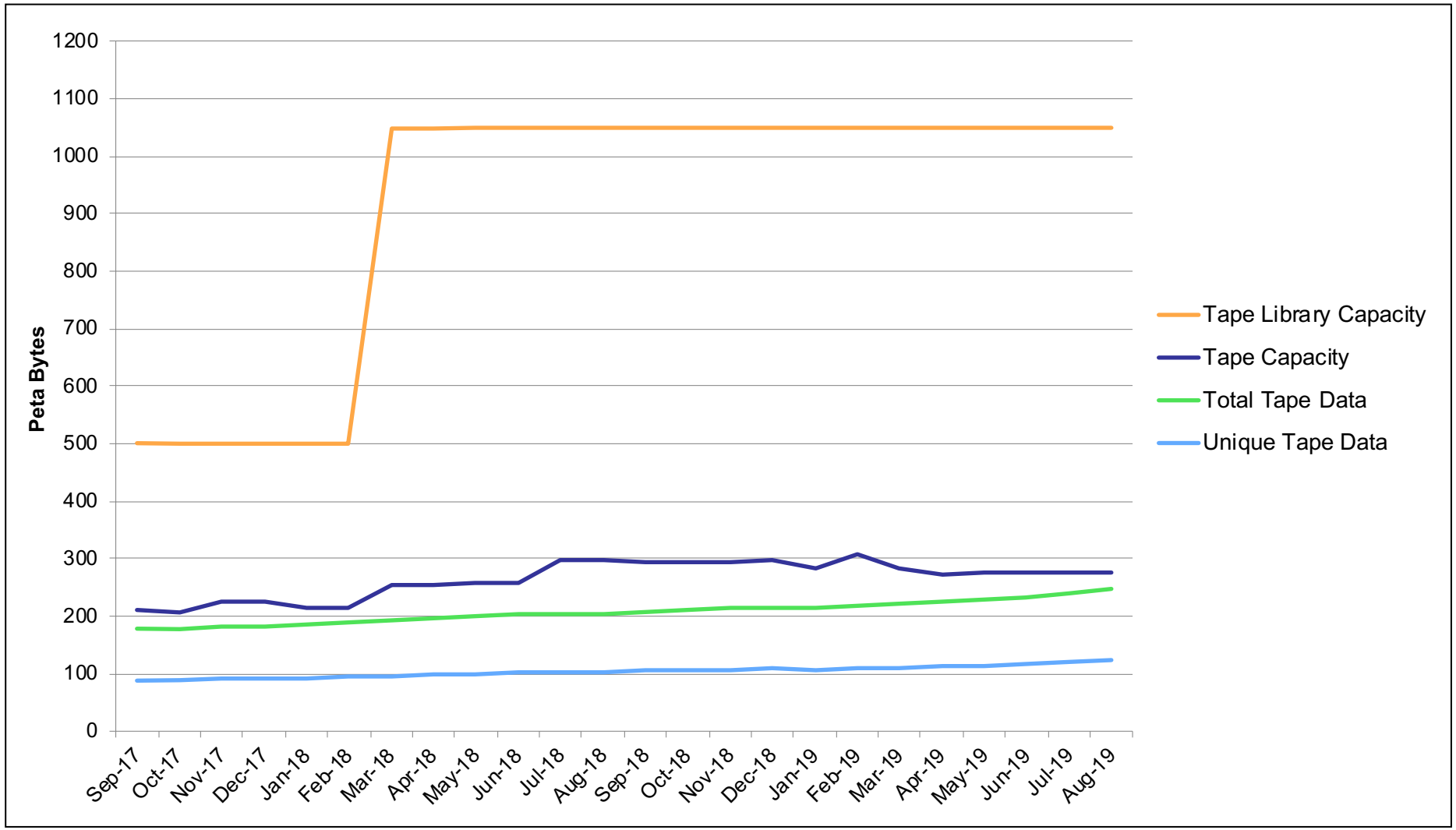
③ 2 Skylake E cells (8 D Rack Equivalence) added to Electra; 1 rack is dedicated to SMD

④ Skylake Tesla GPU V100 Nodes installed

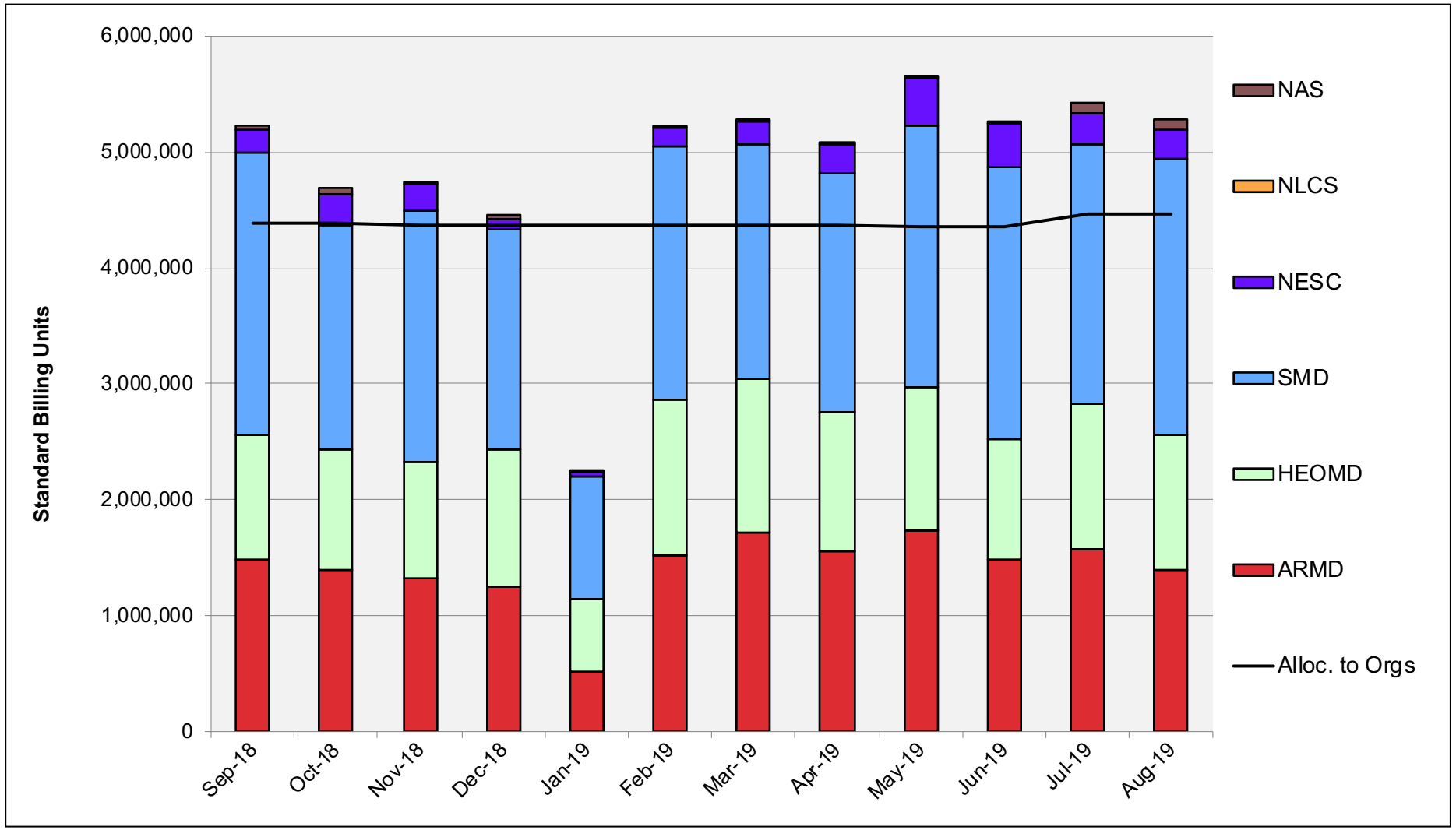
Tape Archive Status



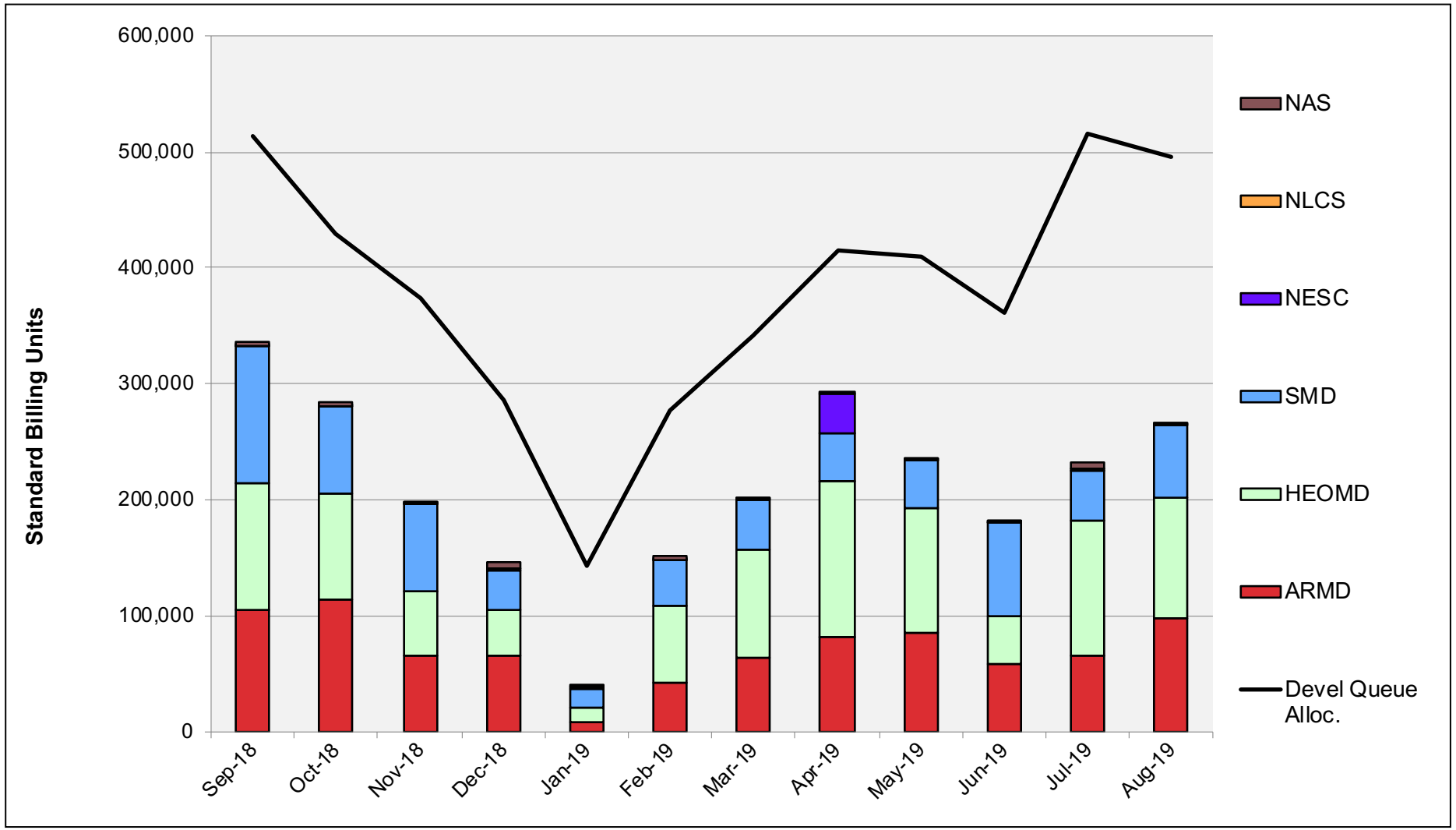
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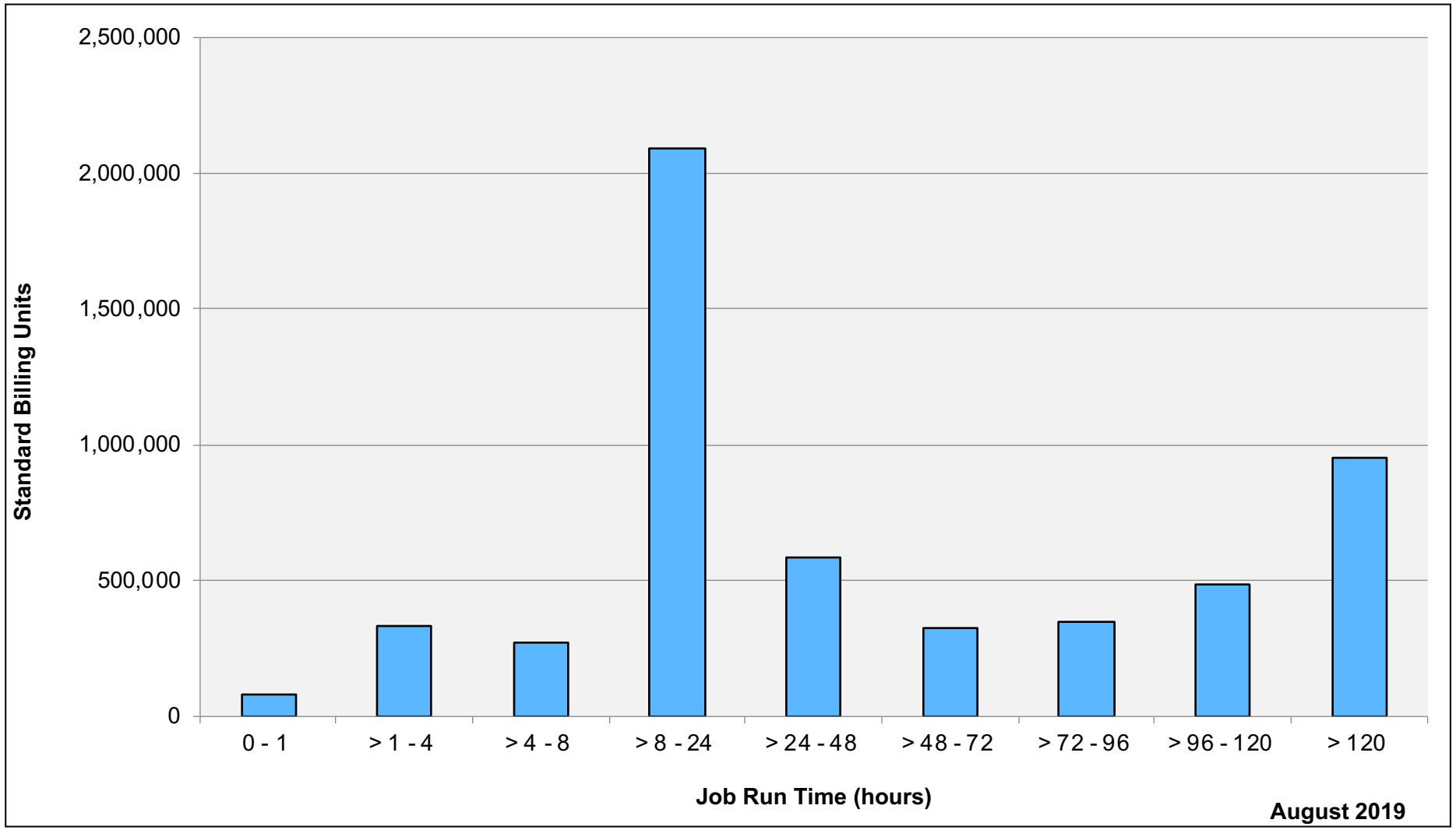
Pleiades: SBUs Reported, Normalized to 30-Day Month



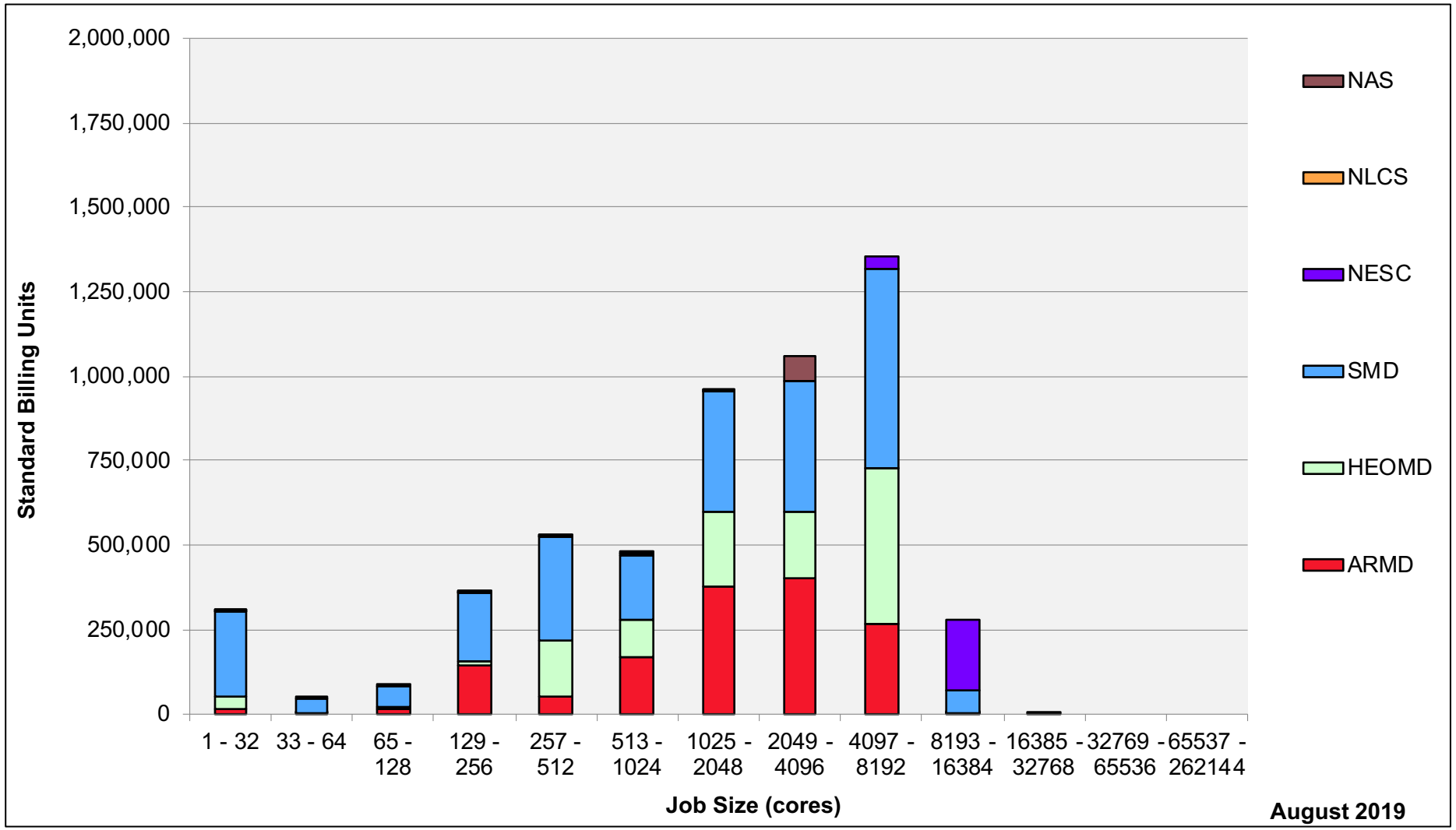
Pleiades: Devel Queue Utilization



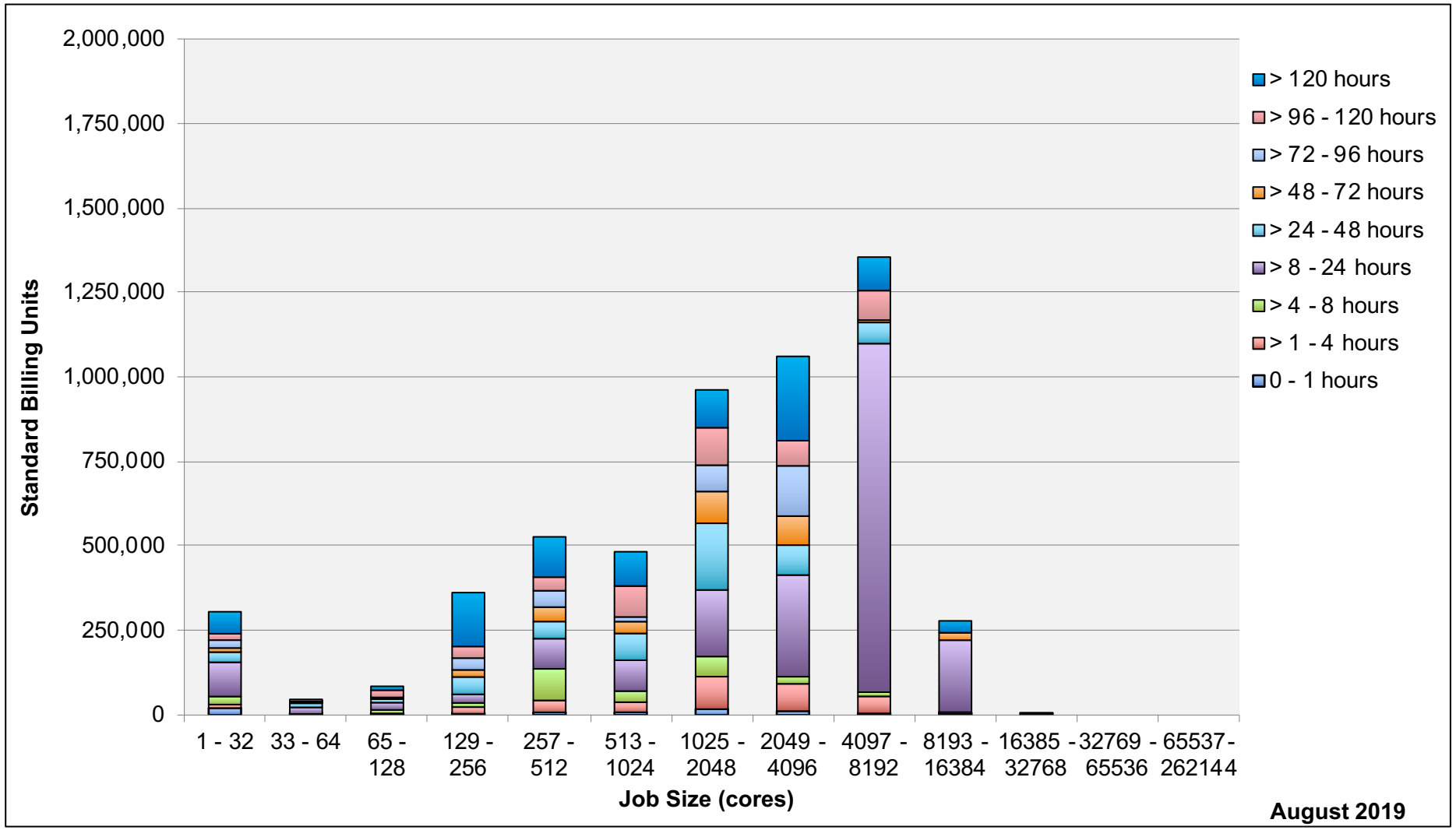
Pleiades: Monthly Utilization by Job Length



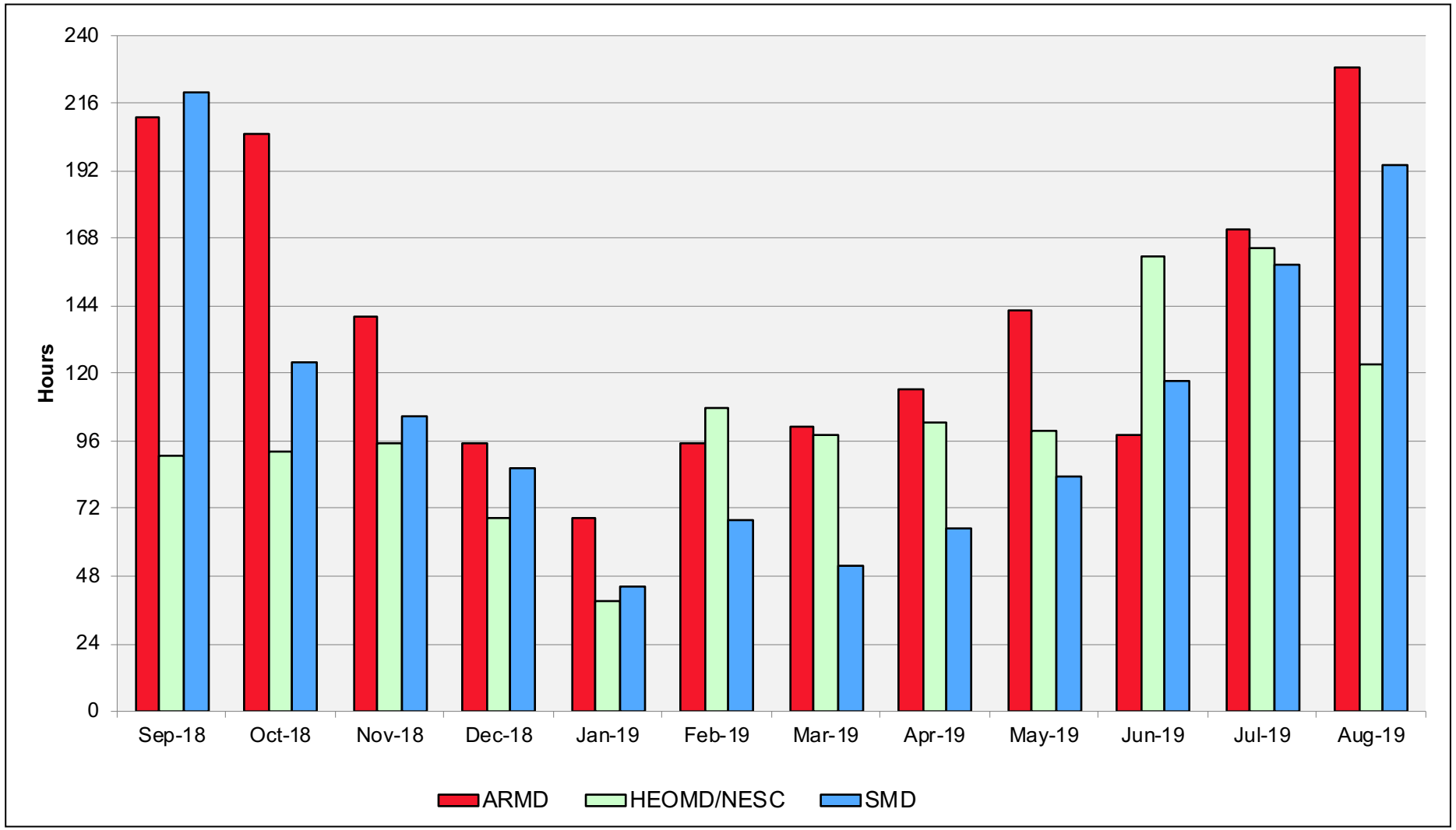
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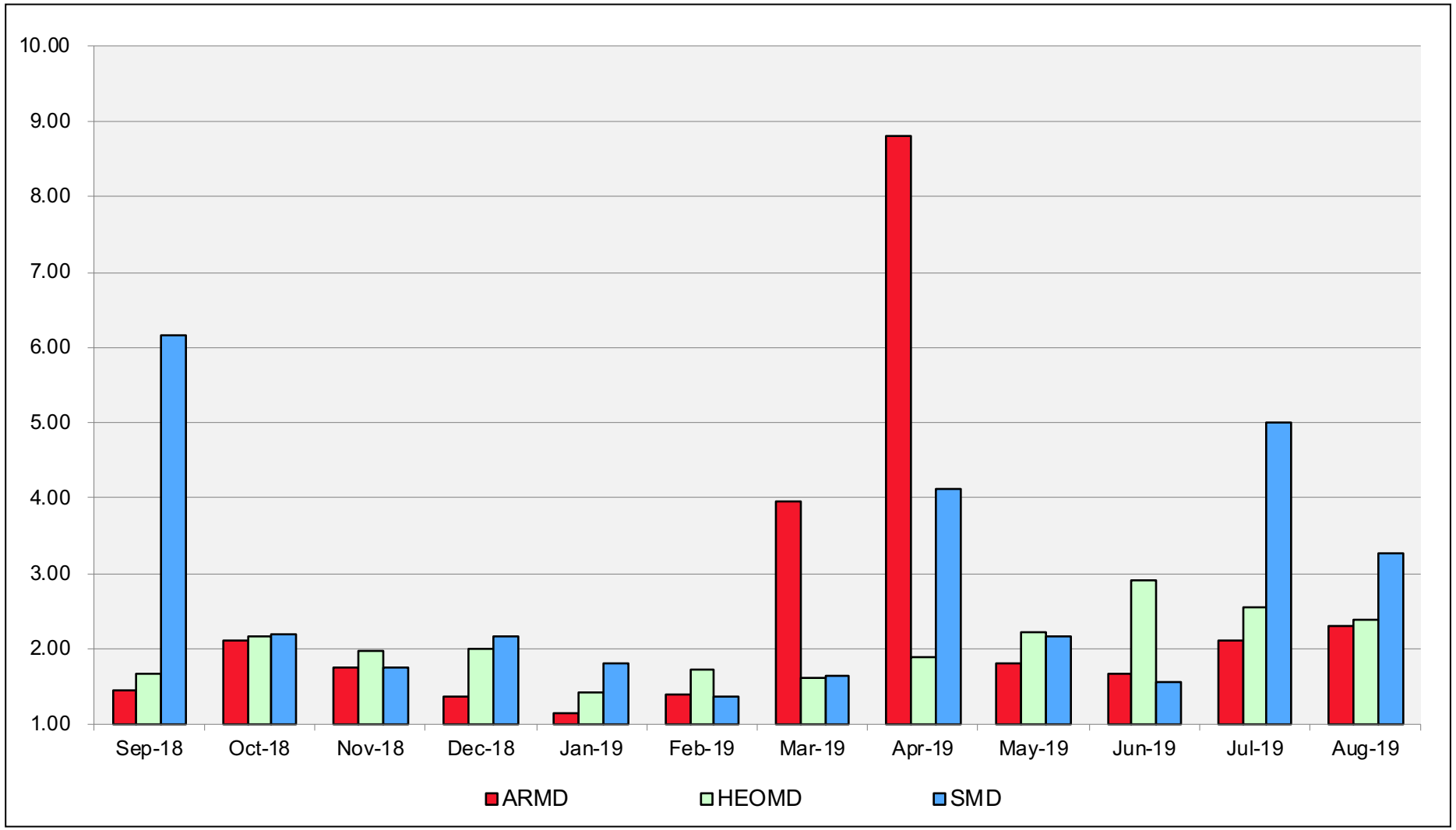
Pleiades: Monthly Utilization by Size and Length



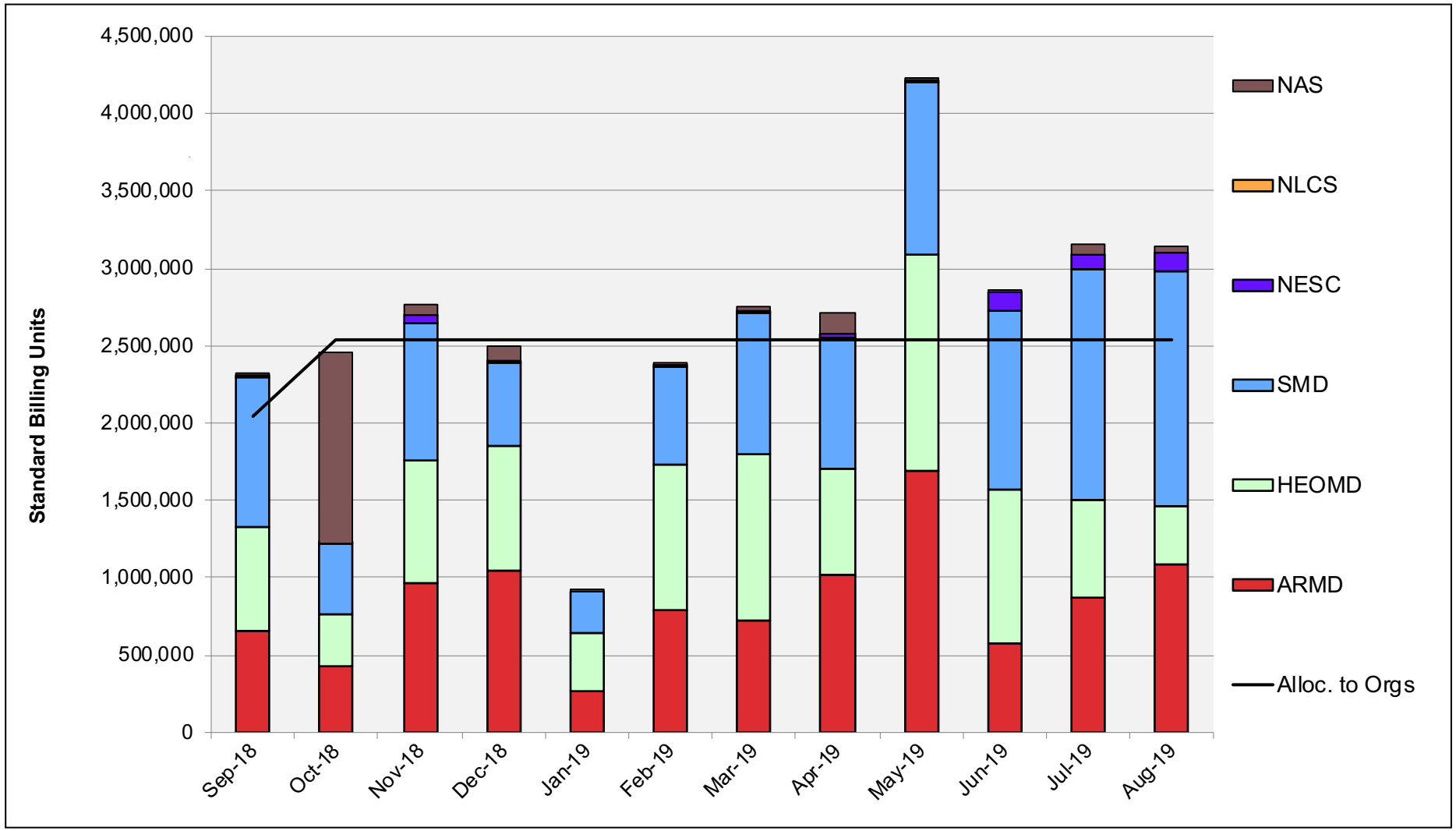
Pleiades: Average Time to Clear All Jobs



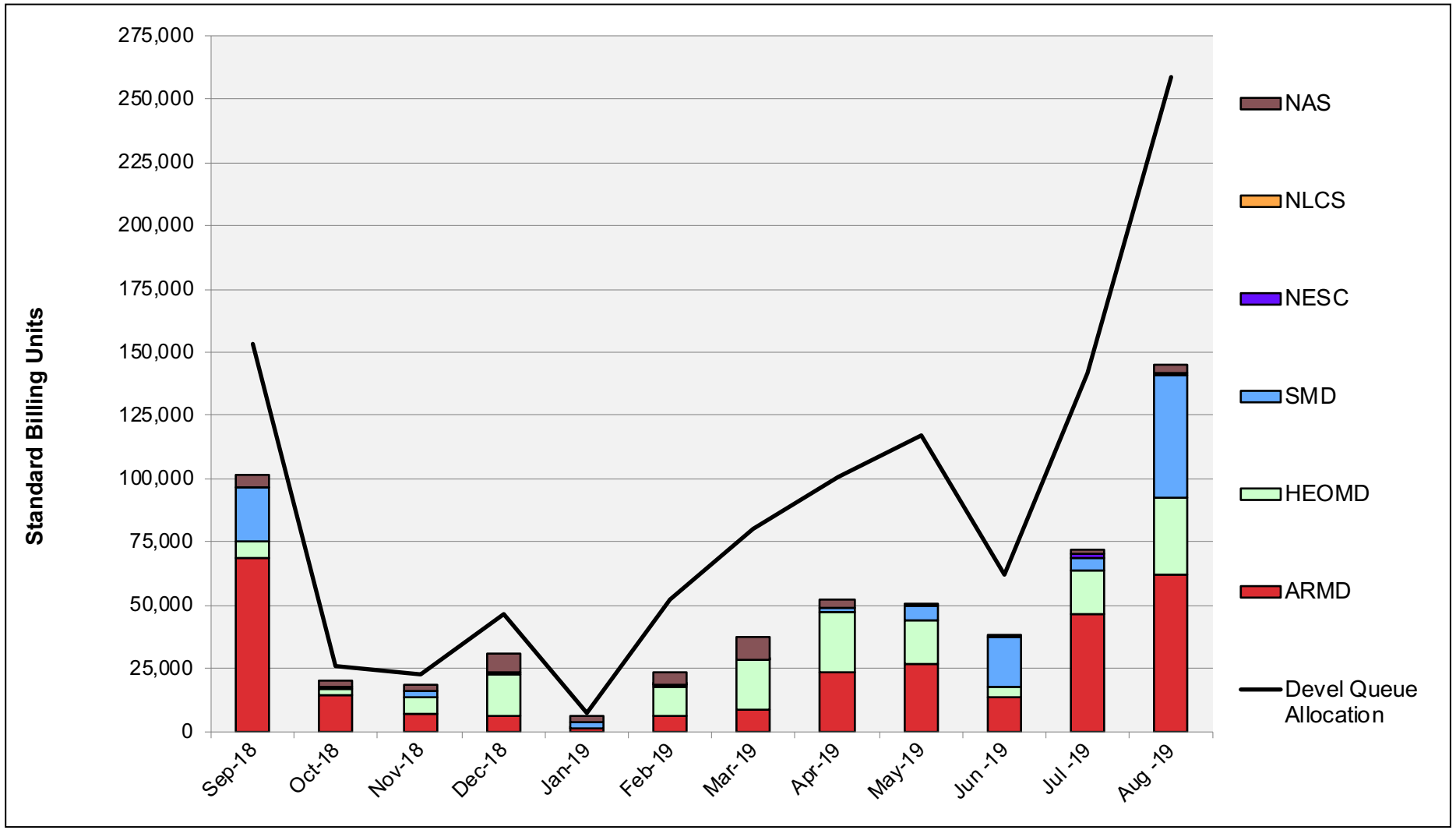
Pleiades: Average Expansion Factor



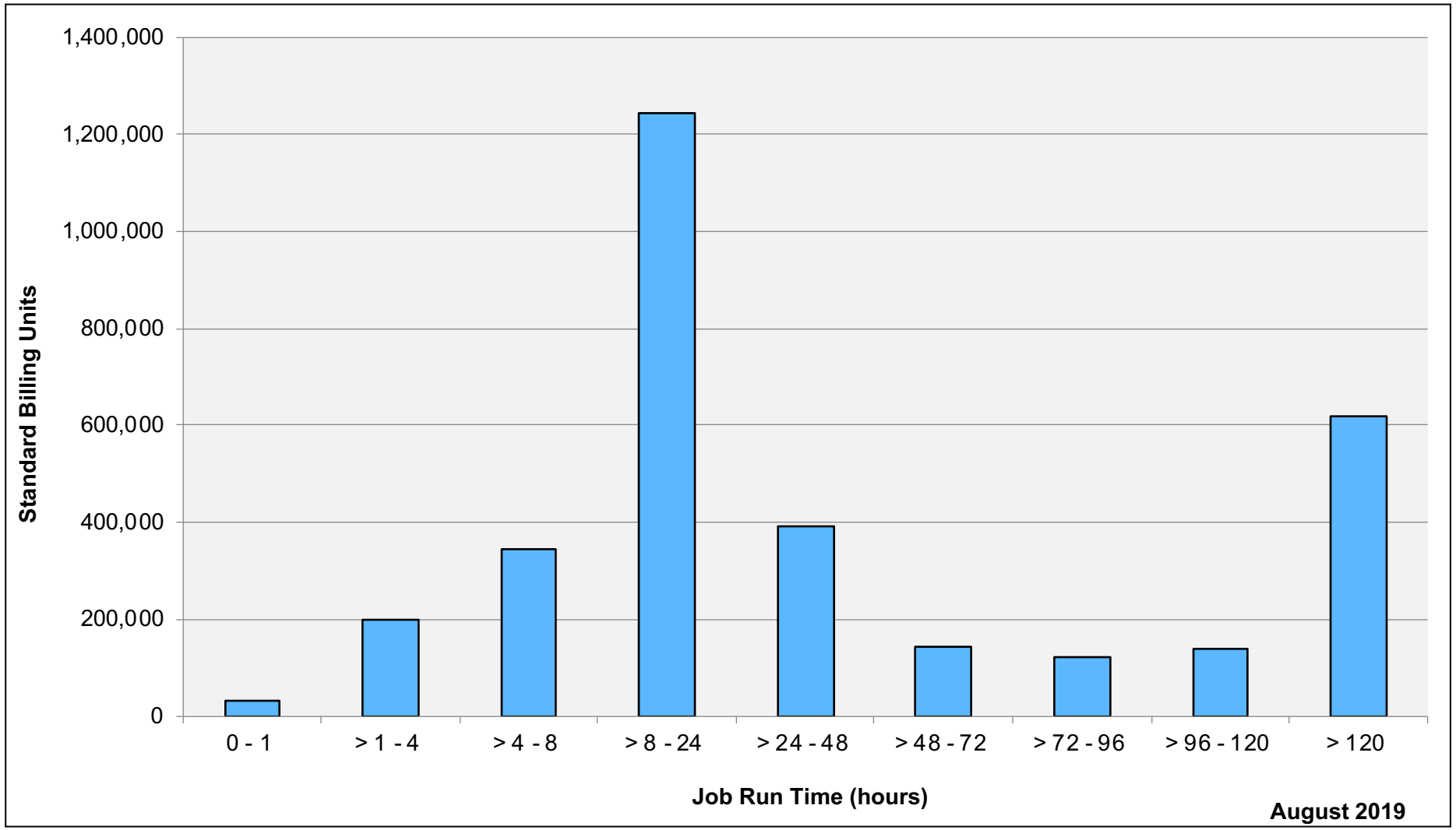
Electra: SBUs Reported, Normalized to 30-Day Month



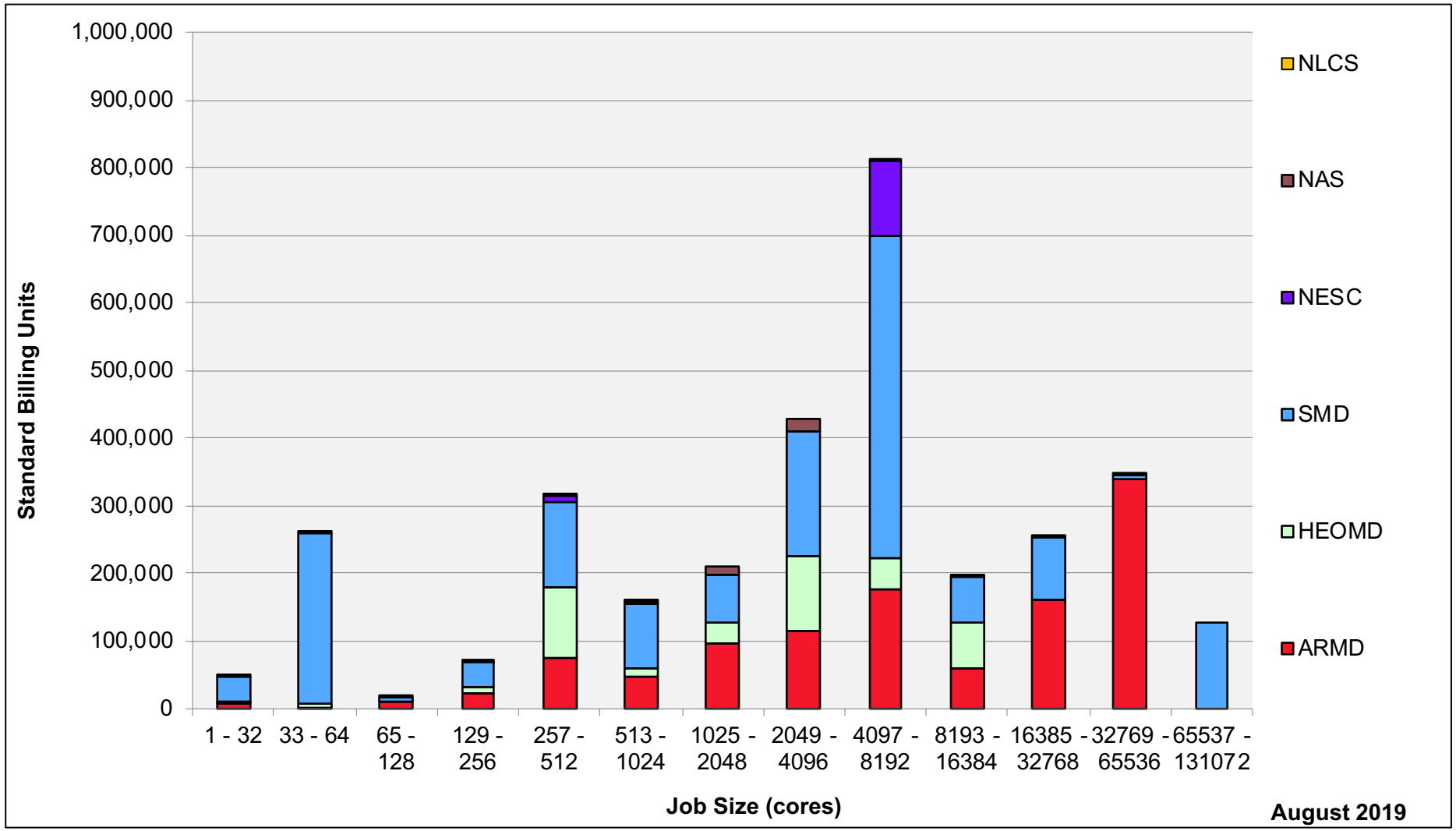
Electra: Devel Queue Utilization



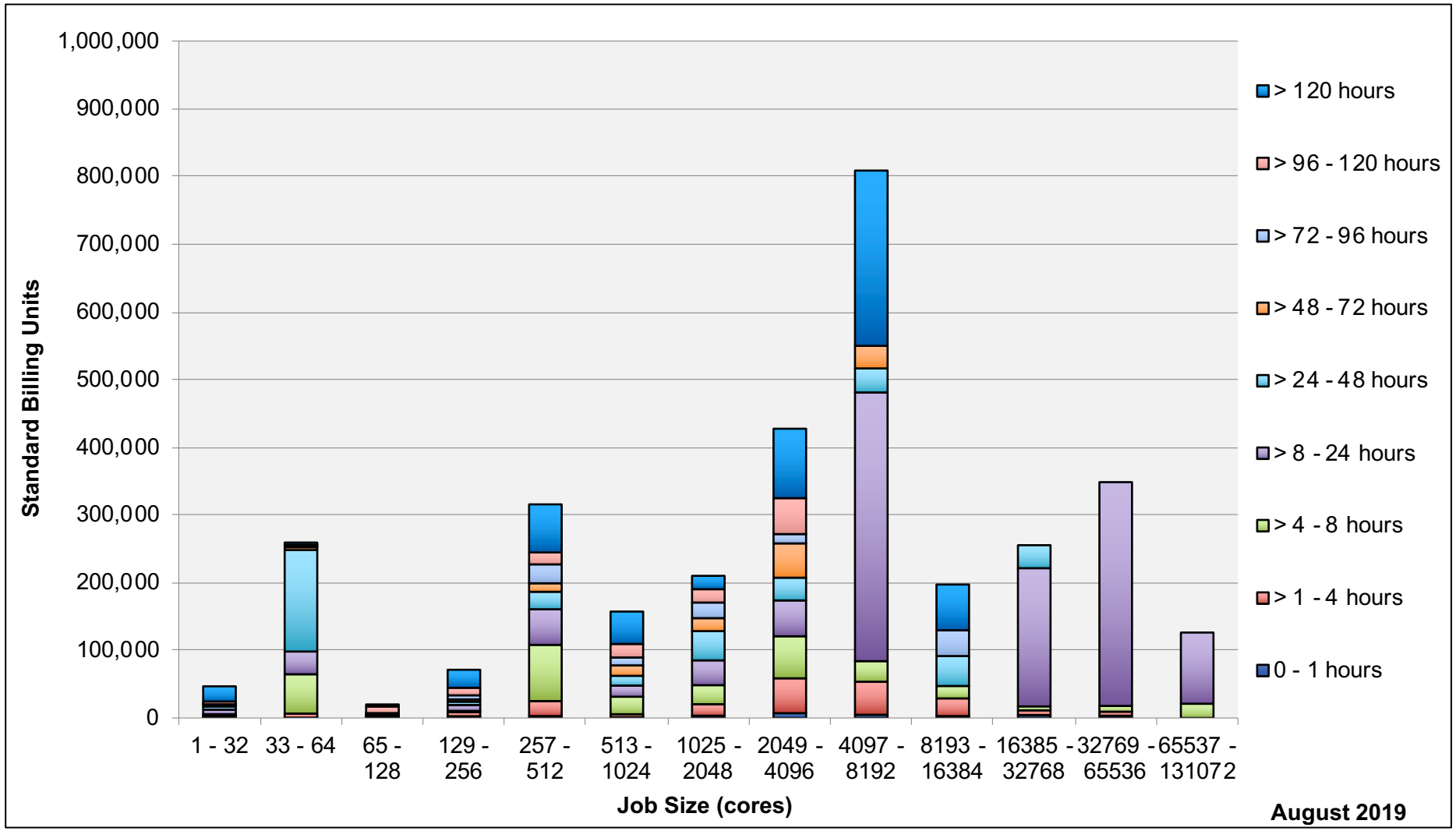
Electra: Monthly Utilization by Job Length



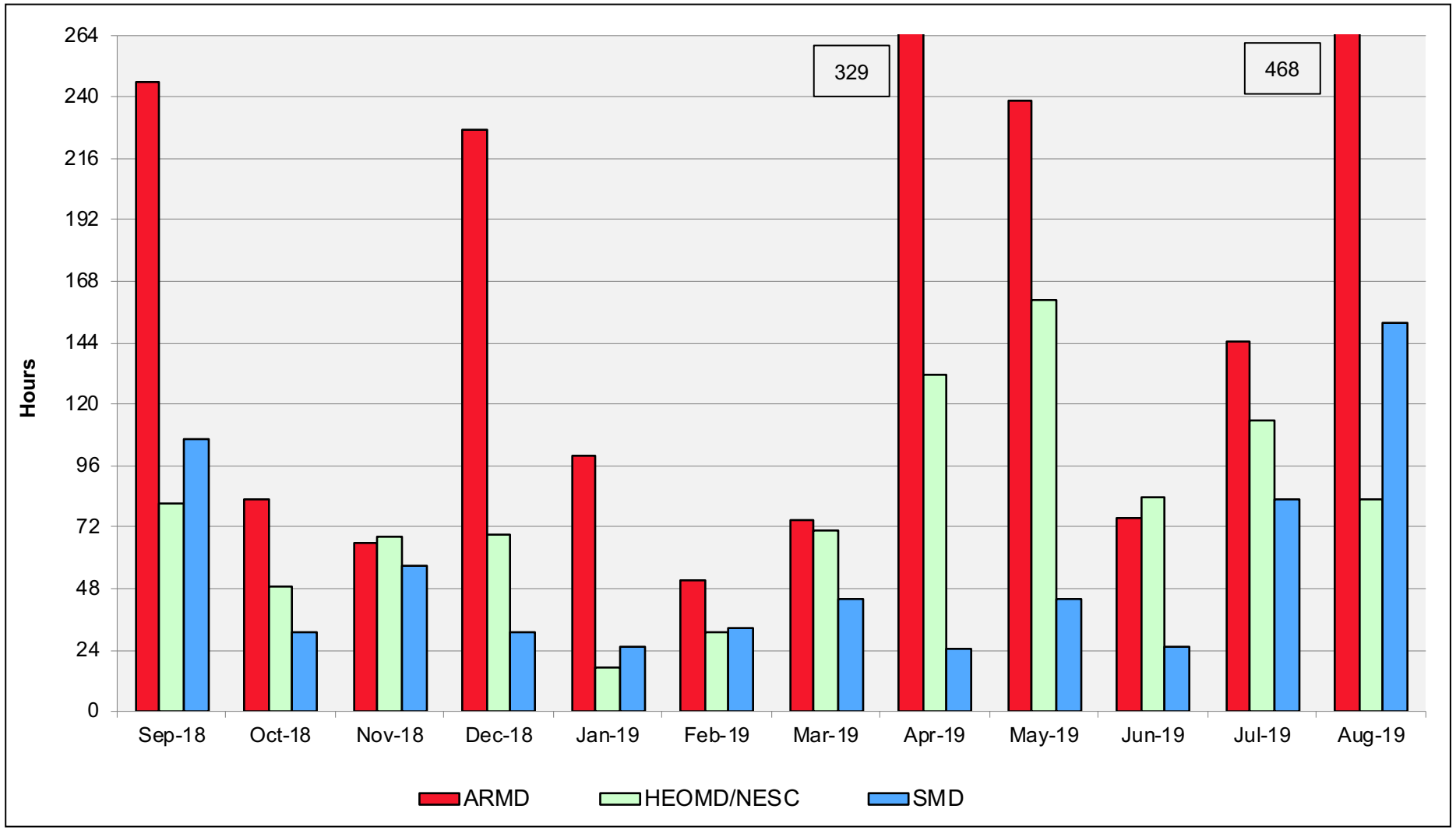
Electra: Monthly Utilization by Job Length



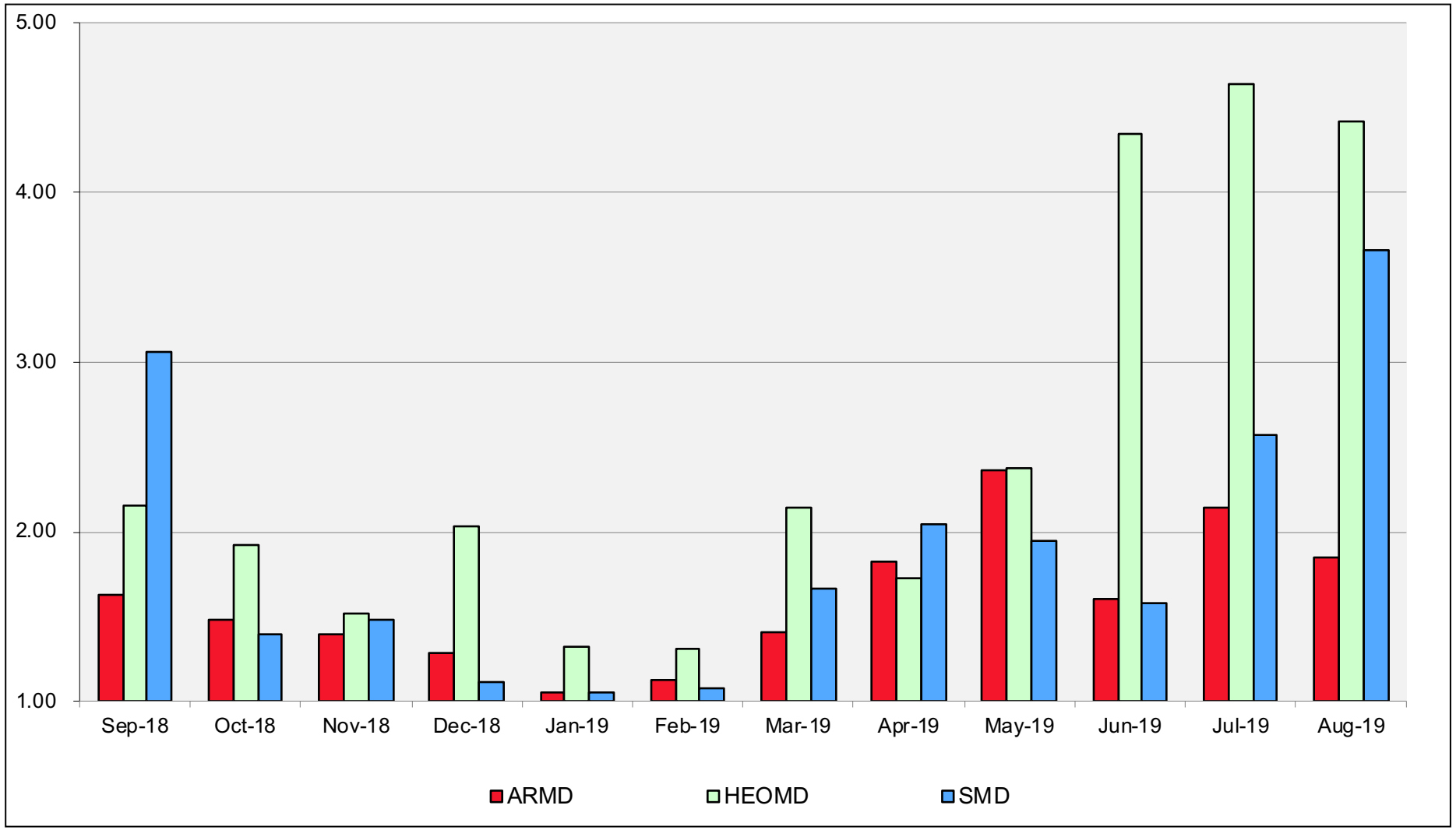
Electra: Monthly Utilization by Size and Length



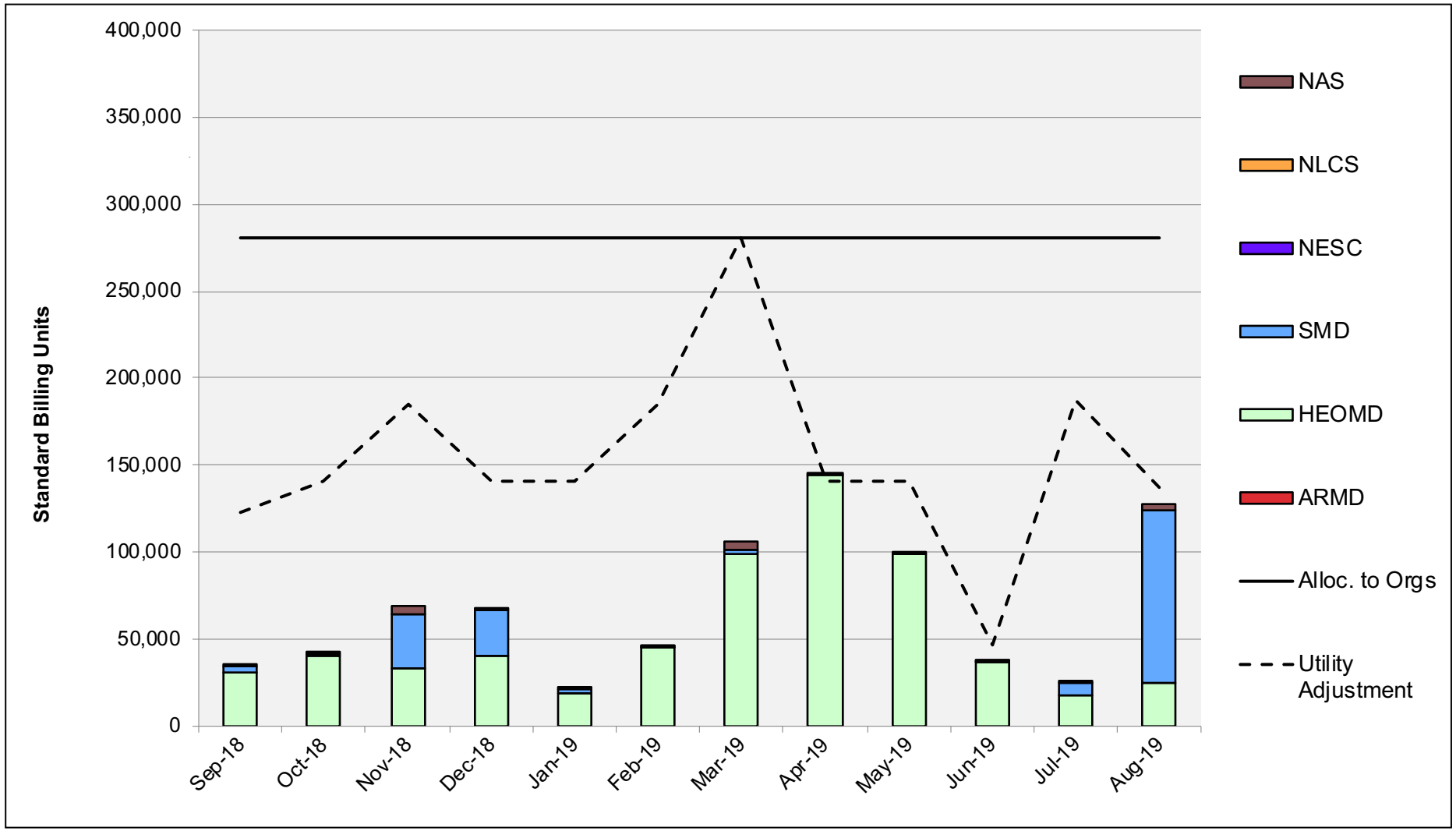
Electra: Average Time to Clear All Jobs



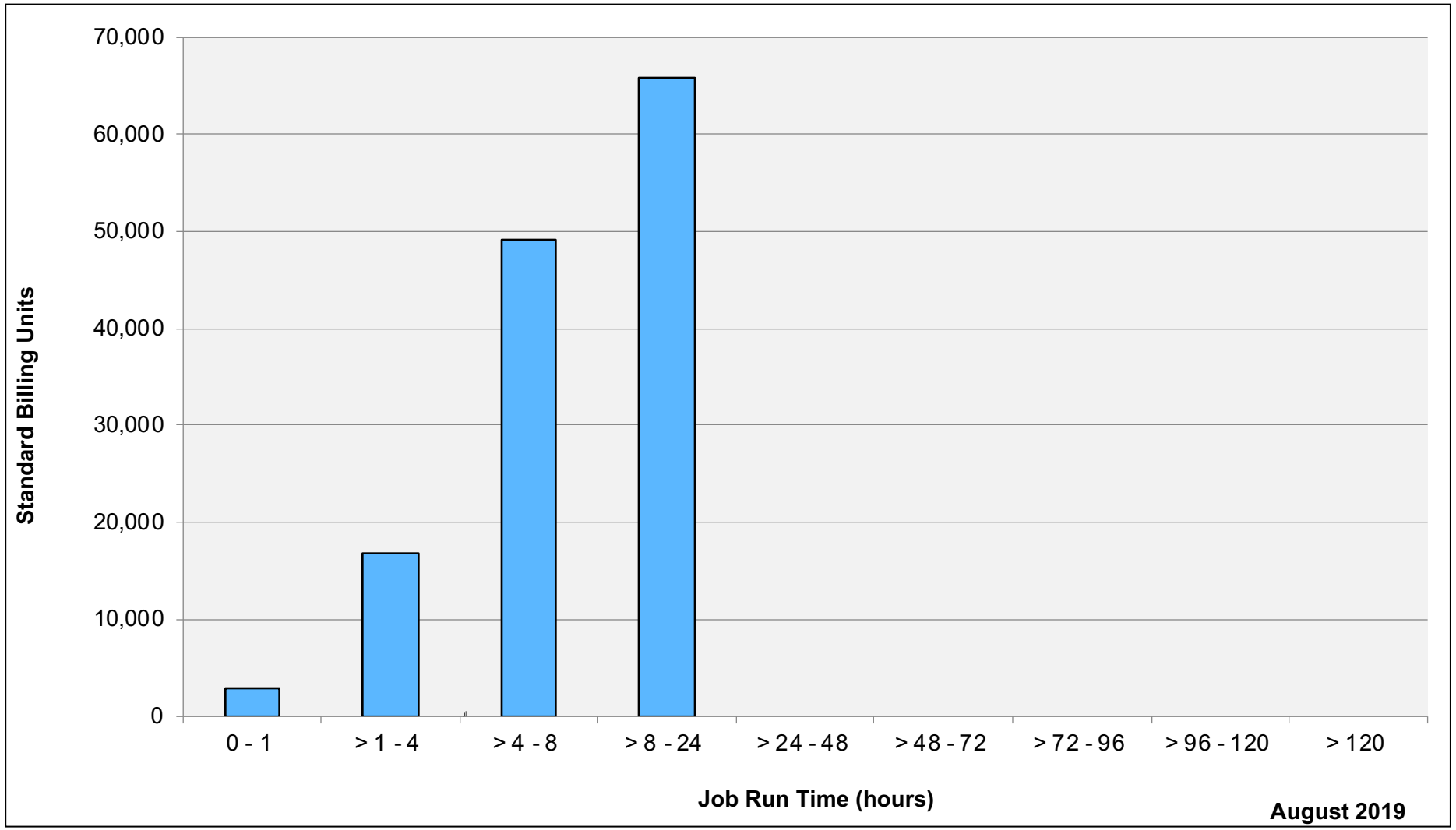
Electra: Average Expansion Factor



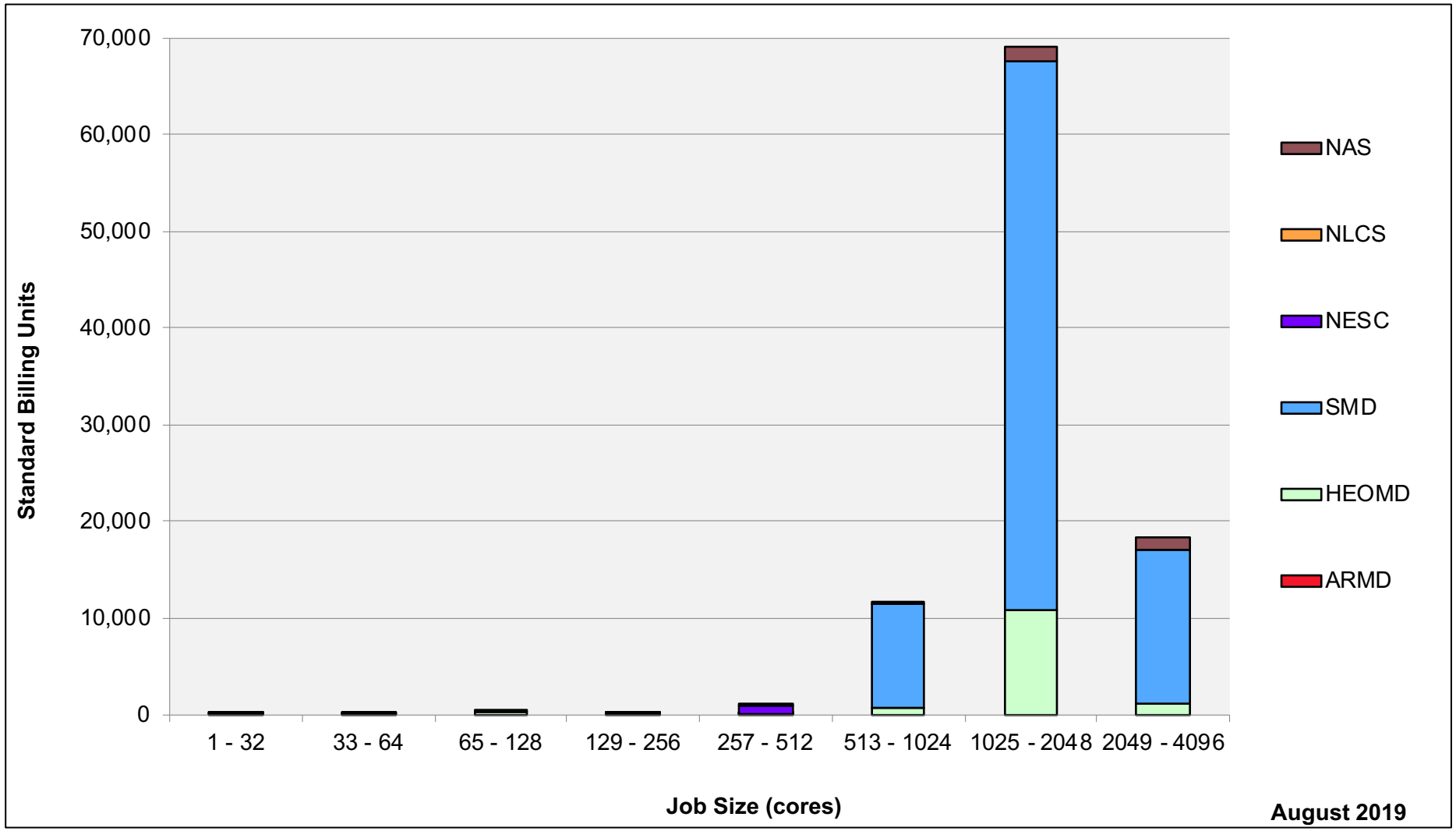
Merope: SBUs Reported, Normalized to 30-Day Month



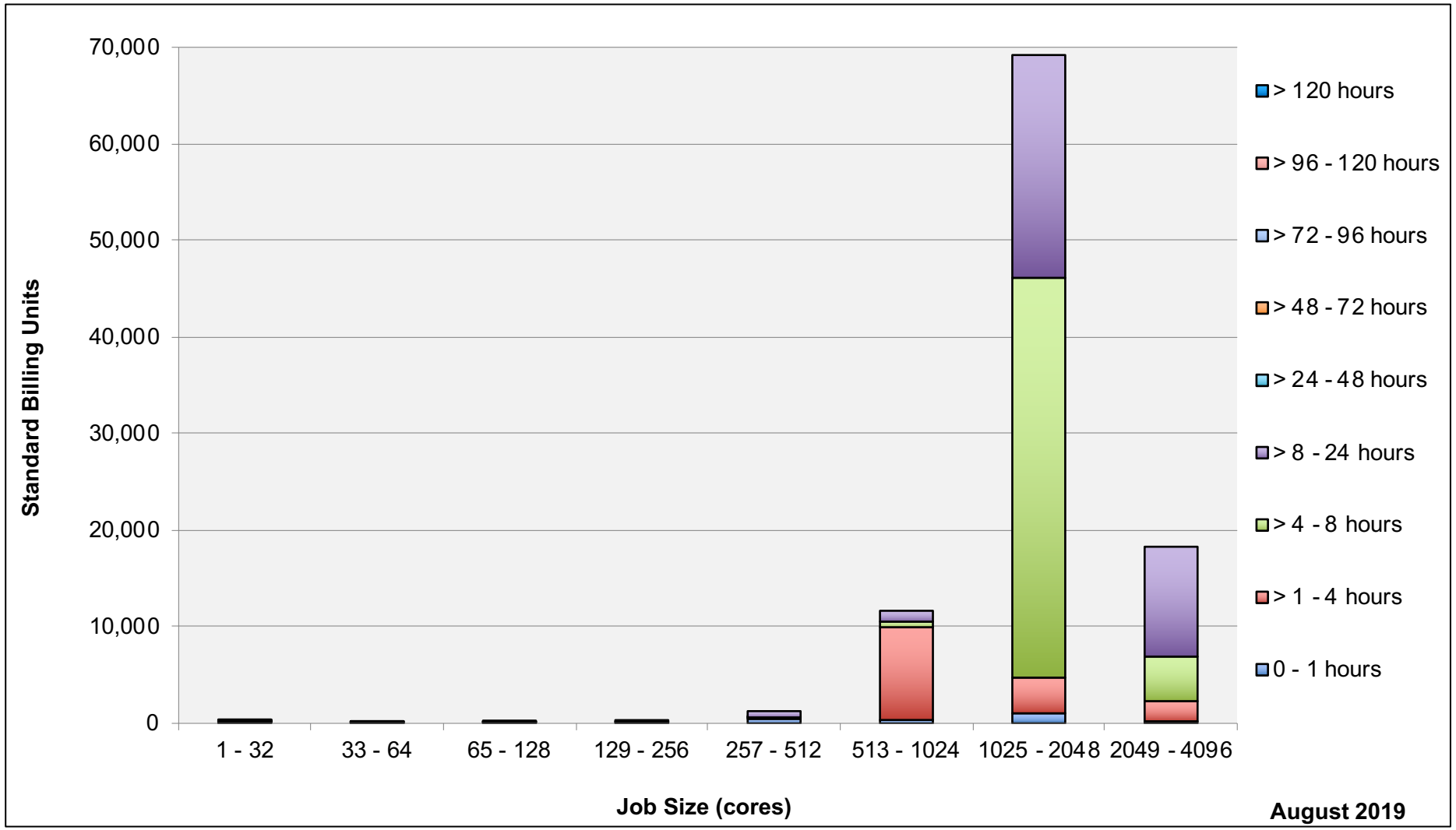
Merope: Monthly Utilization by Job Length



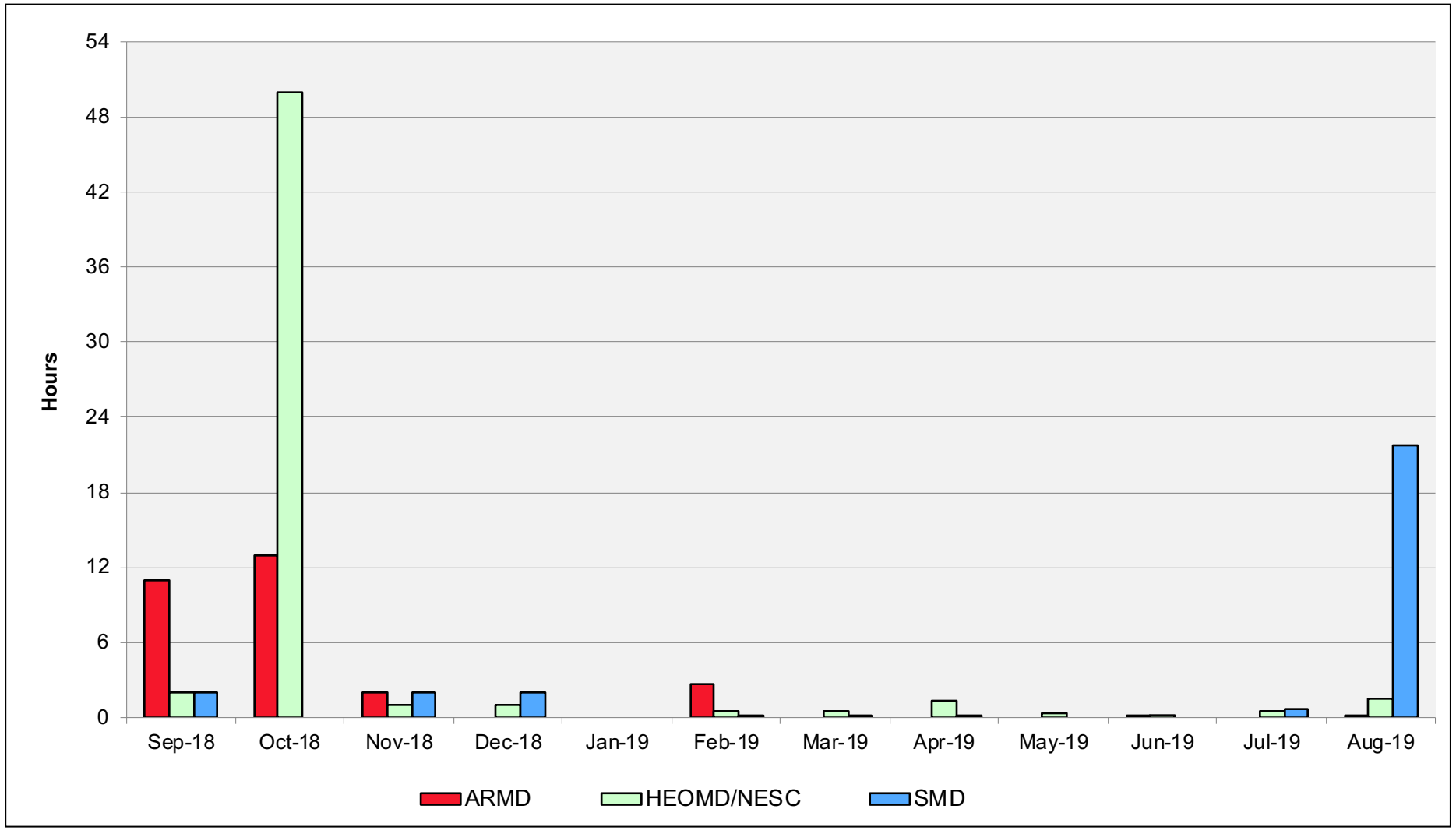
Merope: Monthly Utilization by Job Length



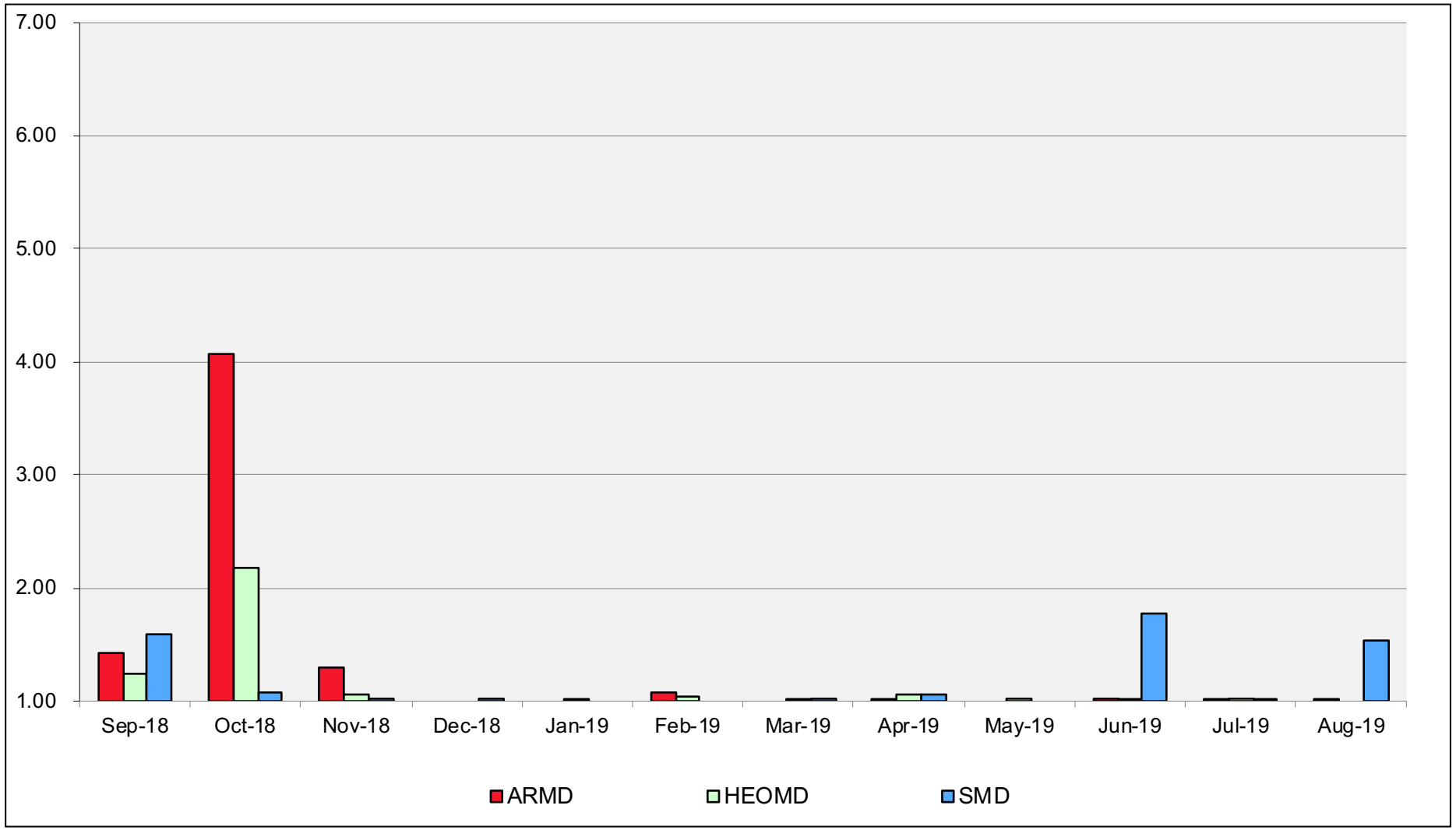
Merope: Monthly Utilization by Size and Length



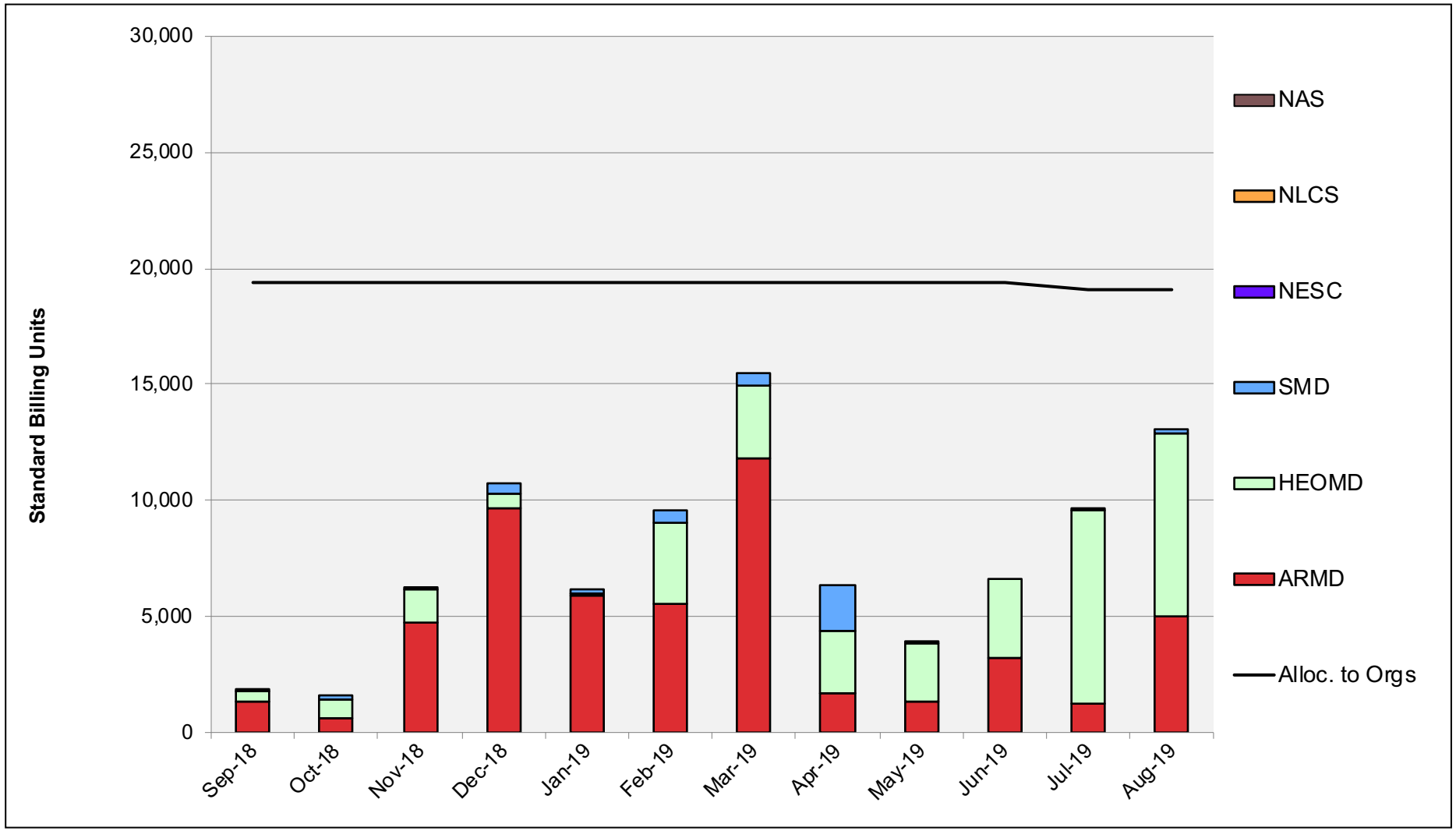
Merope: Average Time to Clear All Jobs



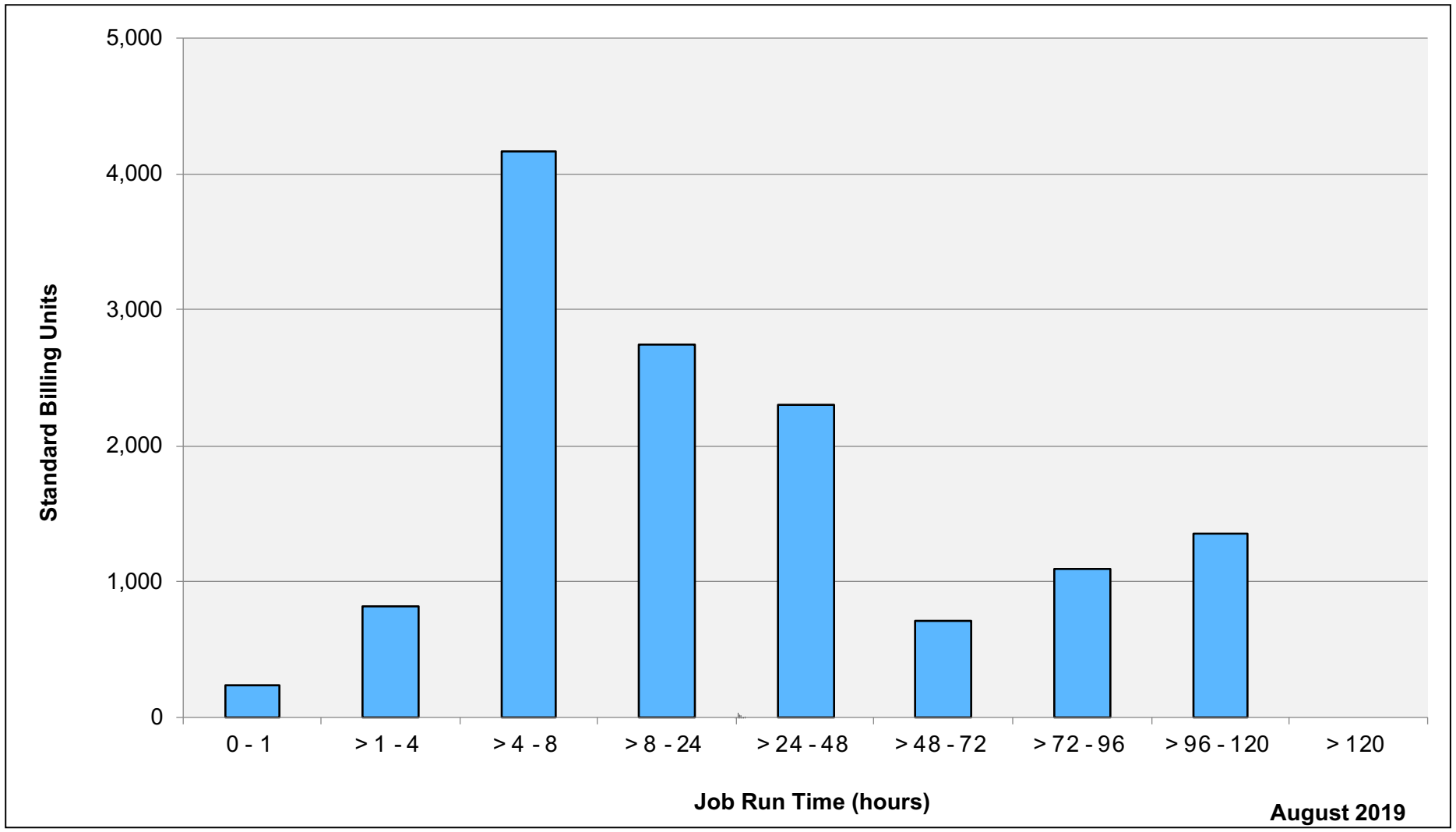
Merope: Average Expansion Factor



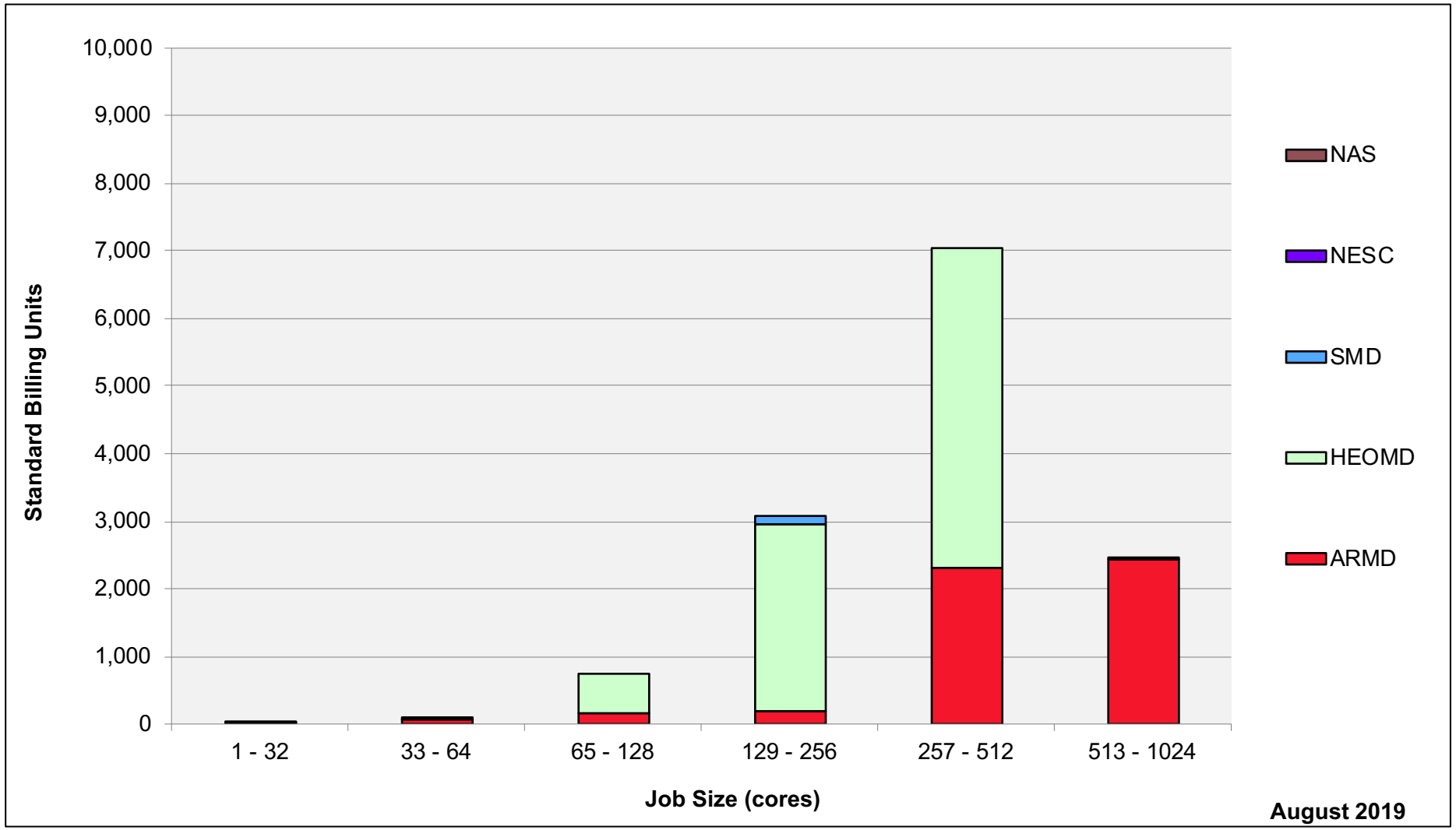
Endeavour: SBUs Reported, Normalized to 30-Day Month



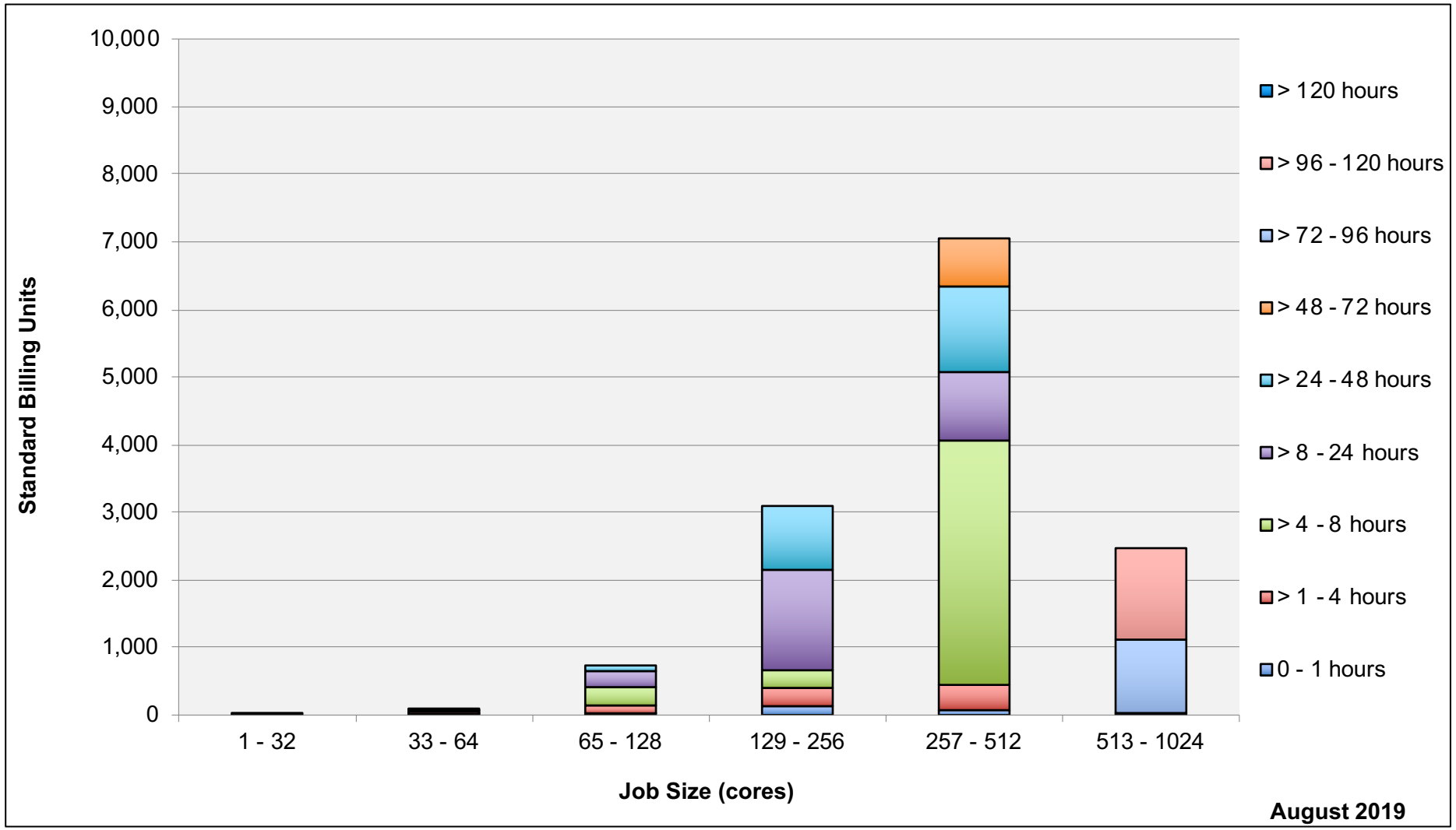
Endeavour: Monthly Utilization by Job Length



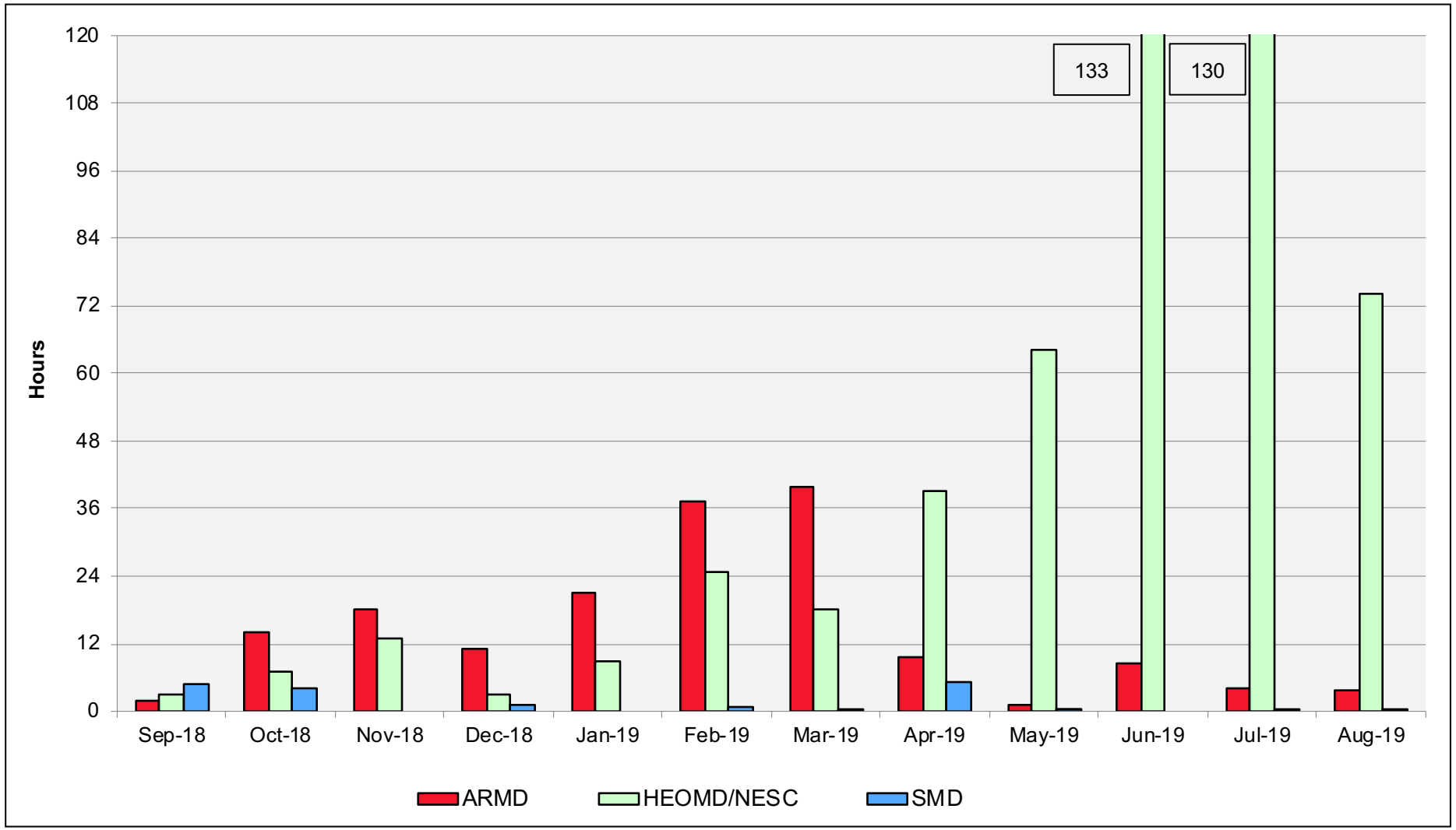
Endeavour: Monthly Utilization by Job Length



Endeavour: Monthly Utilization by Size and Length



Endeavour: Average Time to Clear All Jobs



Endeavour: Average Expansion Factor

