

National Aeronautics and Space Administration

HIGH-END COMPUTING CAPABILITY PORTFOLIO

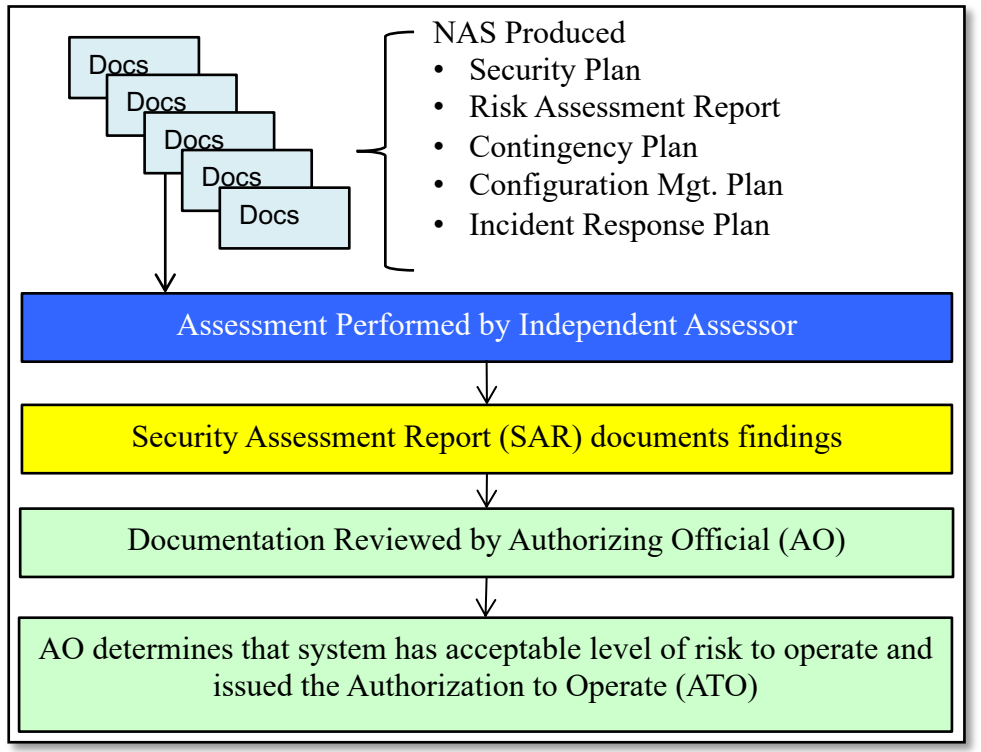
William Thigpen
NASA Advanced Supercomputing Division

October 10, 2021

Independent Assessment of the NAS Security Plan Completed

- The NAS Systems Environment (NSE) System Security Plan (SSP) is in the final year of its triennial assessment and authorization cycle.
- An independent assessment is required under agency policy. The Code 700 Security Controls Assessment team at NASA's Goddard Space Flight Center served as the NSE's independent assessor and issued a Security Assessment Report (SAR). The assessor evaluated the compliance of NSE facilities, systems, and operations, including HECC systems, with agency requirements.
- The SAR is the final step prior to requesting a renewed Authorization to Operate (ATO). Issuance of an ATO will permit NSE and HECC operations for another year, in compliance with NASA security requirements.
- In late October, the HECC security team will meet with the deputy center director at NASA's Ames Research Center, who is the Authorizing Official (AO) for NSE.

IMPACT: Reauthorization of the NAS Systems Security Plan will allow HECC systems to continue operating for another year and continue to provide supercomputing resources to NASA missions, programs, and projects.



Flow chart outlining the evaluation and approval process leading to receiving an Authorization to Operate (ATO).

500x Performance Improvement to Radiative Transfer Code

- The HECC Visualization and Data Analysis team, in support of researchers at the Space Telescope Science Institute (STSci)/ Johns Hopkins University, improved the performance of the PowerDay/Hyperion radiative transfer code by more than 500x.
  - PowerDay consists of several different codes working in a pipeline.
  - The existing PowerDay system would have taken about 9 years of computer time to produce the latest animation.
- The STSci team simulates galaxy formation using ENZO, without an explicit dust model. PowerDay/Hyperion adds a dust model and calculates the transfer of energy to the dust via electromagnetic radiation (radiative transfer). This creates realistic images and spectra that can be used as “virtual observations.”
- The HECC team streamlined the pipeline workflow, producing the latest animation in about one week—a speedup of 500x. They:
  - Reduced duplication and minimized use of HDF5 and Python.
  - Concentrated on the bottlenecks in the Hyperion process.
  - Added a per-node shared memory segment for large read-only data.
  - Rewrote portions of Hyperion to implement OpenMP, allowing the use of all cores on a node with only a modest increase in memory footprint.

IMPACT: Enabled by HECC visualization experts, performance improvements to the radiative transfer workflow will allow researchers to refine and iterate on their methods and models. Existing movies have already provided scientific insight and proven highly effective for conveying results to other scientists and the public.

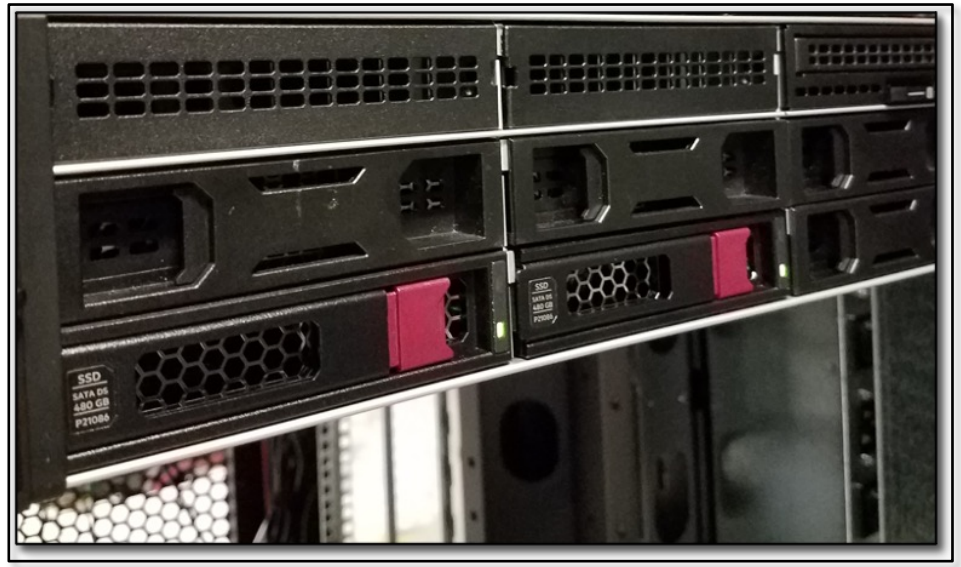


Video of the “Blizzard” simulation showing two interacting galaxies about to collide, and two smaller "satellite" galaxies that are orbiting the main pair. Blue/white glow represents many billions of stars; red/brown shows dust that absorbs light from the stars. Each frame is roughly five million years. *Christopher Henze/NASA Ames*

HECC Tests AMD Instinct MI100 GPU System

- HECC's Systems and Applications teams recently collaborated to complete the evaluation of a single-node system equipped with 2 AMD's MI100 GPUs.
- The Systems team overcame several hurdles to bring the MI100 system online.
  - The MI100 system had to be configured on a specialized network to meet security requirements.
  - The Systems team initially installed the latest version of RHEL, 8.4, but discovered that RHEL 8.3 was needed to support the GPUs.
  - The Systems team worked with AMD to optimize the performance of the GPUs.
- The Applications team ran benchmarks implemented with OpenMP plus Target-offload Directives, including NAS Parallel Benchmarks and a lattice quantum chomodynamics (QCD) mini-application, GridMini. They also ported a global reduction benchmark code, which ran successfully.
- The performance of the MI100 system was encouraging and further study is warranted. The Applications team recommends investigating a multi-node system based on AMD's new MI200 GPU and comparing the performance of that to NVIDIA's A100.

IMPACT: GPU-accelerated systems have the potential to lower the cost of computing for a significant portion of HECC's workload.



HPE installed loaner AMD MI100 GPU-based system at NAS for HECC testing. *Jason Inoue, Unisys*

Testing Period Begins for TOSS 3 Operating System

- HECC prepared for and provided users with testing instructions for a phased transition from the SUSE Linux Enterprise Server (SLES 12 and 15) operating system environment to the Red Hat Enterprise Linux (RHEL)-based Tri-Lab Operating System Stack (TOSS 3). One of the biggest challenges of migrating users to TOSS 3 is making all the software that users depend on work together.
- The goal of the testing effort is to find and fix the bulk of all software compatibility issues for a seamless transition.
- The APP group ran all SBU1 benchmarks to verify functionality.
  - Existing SLES12 executables and the most commonly used dependent libraries (hdf4/hdf5/netcdf) from SLES 12 can be used in the TOSS 3 environment as-is, with no need to rebuild any libraries or executables.
  - NVIDIA's HPC Software Development Kit and profiling tools (nsys and ncu) work under TOSS 3. (The SLES 12-built NVIDIA compilers and toolkit were reinstalled with the RHEL counterparts.)
- Cases found where transition isn't seamless, with solutions:
  - If using SGI/HPE MPT older than MPT 2.23 on SLES 12, users need to load the newer MPT 2.23; no need to recompile.
  - The SLES 12 petsc data structures and routines were rebuilt for TOSS 3.
  - The SLES 12-built version of libstdc++.so.6 fails because this executable depends on GLIB_2.18. The TOSS 3 version of /lib/libc.so.6 only goes up to GLIBC_2.17. Putting the TOSS 3-built version of libstdc++.so.6 ahead in the search path solves this problem.

IMPACT: Migrating to TOSS 3, which is optimized for high-performance computing clusters, can reduce total cost of ownership, enable application portability, and ensure timely access to security patches. The extensive testing process will help ensure users' applications will continue to run by December, when the TOSS 3 environment will be in full production.



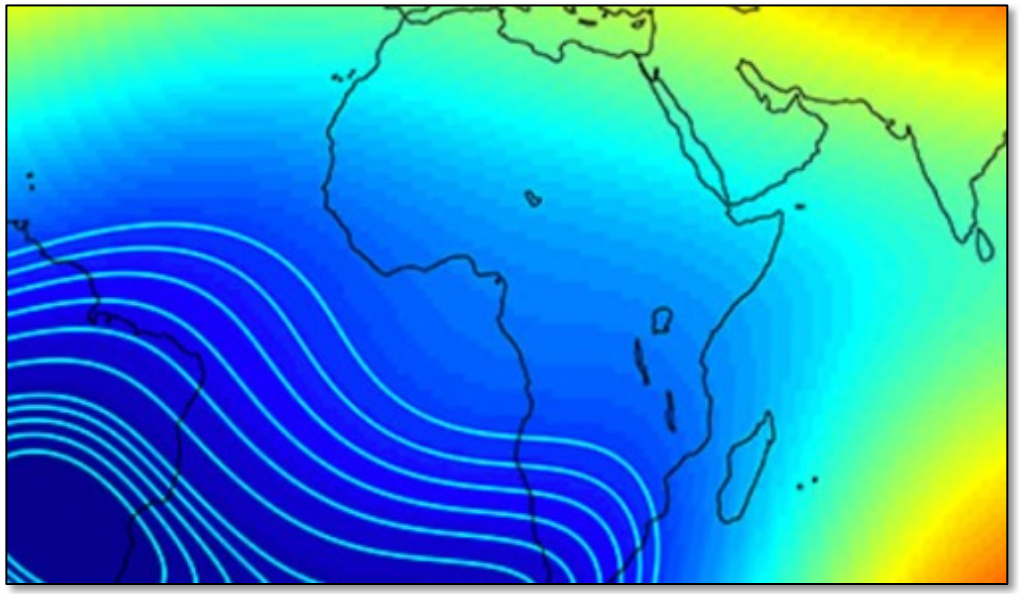
The original TOSS environment effort was led by Lawrence Livermore National Laboratory (LLNL), and was built as a common capacity hardware environment, called the Tri-Lab Linux Capacity Clusters (TLCC1), at the three National Nuclear Security Administration laboratories: LLNL, Los Alamos, and Sandia.

Predicted Expansion of the South Atlantic Anomaly Enabled by HECC Resources

- A collaborative team at NASA Goddard and the University of Maryland, Baltimore County is working to better estimate the dynamic core state and predict variations in Earth's magnetic field.
- As part of the geomagnetic data assimilation (GDAS) project, the team used the Geomagnetic Ensemble Modeling System (GEMS) tool to make forecasts until the next analysis time. Much of the computation was done on the Pleiades supercomputer.
  - The team produced two animations of the geomagnetic intensity variation from 2010 to 2025, one on the Earth's mean surface, the other on the core-mantle boundary (CMB) that is nearly 3,000 kilometers below the surface.
- The team predicted the continued westward expansion of the South Atlantic Anomaly (SAA), an area at the Earth's surface where the geomagnetic field intensity is exceptionally low.
  - The field intensity of the SAA will continue to decrease, and a second minimum will reappear near the end of the forecast period.
  - The SAA provides unique opportunities for studying Earth's deep interior. It is also a geomagnetic hazard to low-Earth orbit space missions and is important to monitor and understand for fundamental science research and societal applications.

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

IMPACT: Monitoring, interpreting, and predicting variations in Earth's magnetic field are critical for understanding the dynamics of our planet's deep interior and interactions between the fluid core and the other Earth systems. HECC resources are critical to the success of this work.



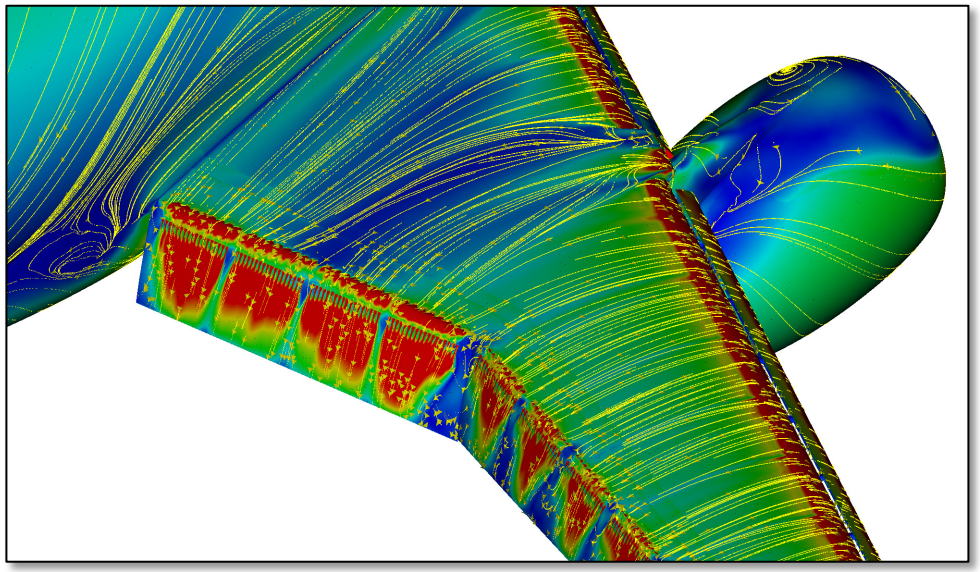
A snapshot of the magnetic field intensity at the Earth's core-mantle boundary (CMB) in 2010–2025. The intensity increases in magnitude from blue (low intensity) to red (high intensity). *Weijia Kuang, NASA/Goddard; Andrew Tangborn, University of Maryland, Baltimore County*

Designing Active Flow Control Actuators for High-Lift Aircraft Design*

- Under the Advanced Air Transportation Technology Project, researchers at NASA's Langley Research Center are examining various approaches to reduce the cruise drag and fuel burn associated with modern high-lift aircraft designs without sacrificing performance during takeoff and landing. An active flow control (AFC) system could provide the required lift when needed, while reducing the possible cruise drag associated with external mechanisms.
- The multi-year effort designed and tested two high-lift configurations of the Common Research Model (CRM); and an AFC-enabled simple-hinged flap configuration was developed to produce a lift coefficient comparable to a conventional high-lift configuration. Using the Lattice-Boltzmann-based flow solver PowerFlow, the team examined the effect of geometric size and placement of rows of sweeping jet and steady blowing jet actuators in order to assess the lift augmentation potential of different arrangements.
- The predictions for lift augmentation with variation in actuation levels were verified by wind tunnel test data. A combination of sweeping jets and steady blowing jets on the AFC-enabled configuration was able to match or exceed the lift coefficient of the conventional high-lift model over a broad range.
- This study required many complex simulations, with a typical medium resolution grid case running on 2,520 Skylake cores over 240 hours on the Electra supercomputer.

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

IMPACT: This work demonstrates the capability of CFD tools and methodologies for conducting parametric studies on complex, high-lift aircraft wing configurations using embedded AFC actuators, as well as helping the design of future aircraft prior to expensive experimental work.



Visualization showing the mitigation of separated flow on the CRM high-lift wing configuration with an active flow control system. Surface color indicates skin friction along the wing during high-lift maneuvers (blue is low, red is high). The yellow lines represent surface streamlines. *Veer Vatsa, NASA/Langley*

Papers

- "**Radiative MHD Simulations of Photon Bubbles in Radiation-Supported Magnetized Atmospheres of Neutron Stars with Isotropic Thomson Scattering**," L. Zhang, O. Blaes, Y.-F. Jiang, Monthly Notices of the Royal Astronomical Society, vol. 508, issue 1, published online September 7, 2021. *
  https://academic.oup.com/mnras/article-abstract/508/1/617/6366253
- "**The TESS Mission Target Selection Procedure**," M. Fausnaugh, et al., Publications of the Astronomical Society of the Pacific, vol. 133, no. 1027, September 8, 2021. *
  https://iopscience.iop.org/article/10.1088/1538-3873/ac1d3f/meta
- "**Flares, Rotation, and Planets of the AU Mic System from TESS Observations**," E. Gilbert, et al., arXiv:2109.03924 [astro-ph.EP], September 8, 2021. *
  https://arxiv.org/abs/2109.03924
- "**The Obliquity of HIP 67522 b: a 17 Myr old Transiting Hot Jupiter-sized Planet**," A. Heitzmann, et al., arXiv:2109.04174 [astro-ph.EP], September 9, 2021. *
  https://arxiv.org/abs/2109.04174
- "**Turbulent Chemical-Species Mixing in the Venus Lower Atmosphere at Different Altitudes: A Direct Numerical Study Relevant to Understanding Species Spatial Distribution**," S. Morellina, J. Bellan, Icarus, published online September 10, 2021. *
  https://www.sciencedirect.com/science/article/abs/pii/S0019103521003420

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

Papers (cont.)

- "**Impact of Subglacial Freshwater Discharge on Pine Island Ice Shelf**," Y. Nakayama, C. Cai, H. Seroussi, Geophysical Research Letters, v. 48, issue 18, September 13, 2021. *
  https://agupubs.onlinelibrary.wiley.com/doi/abs/10.1029/2021GL093923
- "**Radiation GRMHD Simulations of the Hard State of Black Hole X-ray Binaries and the Collapse of a Hot Accretion Flow**," J. Dexter, N. Scepi, M. Begelman, arXiv:2109.06239 [astro-ph.HE], September 13, 2021. *
  https://arxiv.org/abs/2109.06239
- "**Role of Mixed-Layer Instabilities in the Seasonal Evolution of Eddy Kinetic Energy Spectra in a Global Submesoscale Permitting Simulation**," H. Khatri, et al., Geophysical Research Letters, vol. 48, issue 18, September 13, 2021. *
  https://agupubs.onlinelibrary.wiley.com/doi/abs/10.1029/2021GL094777
- "**Bursty Magnetic Reconnection at the Earth's Magnetopause Triggered by High-Speed Jets**," J. Ng, et al., Physics of Plasmas, vol. 28, issue 9, September 13, 2021. *
  https://aip.scitation.org/doi/10.1063/5.0054394
- "**Exosphere Modeling of Proxima b: A Case Study of Photochemical Escape with a Venus-like Atmosphere**," Y. Lee, C. Dong, V. Tenishev, arXiv:2021.06963 [astro-ph.EP], September 14, 2021. *
  https://arxiv.org/abs/2109.06963

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

Papers (cont.)

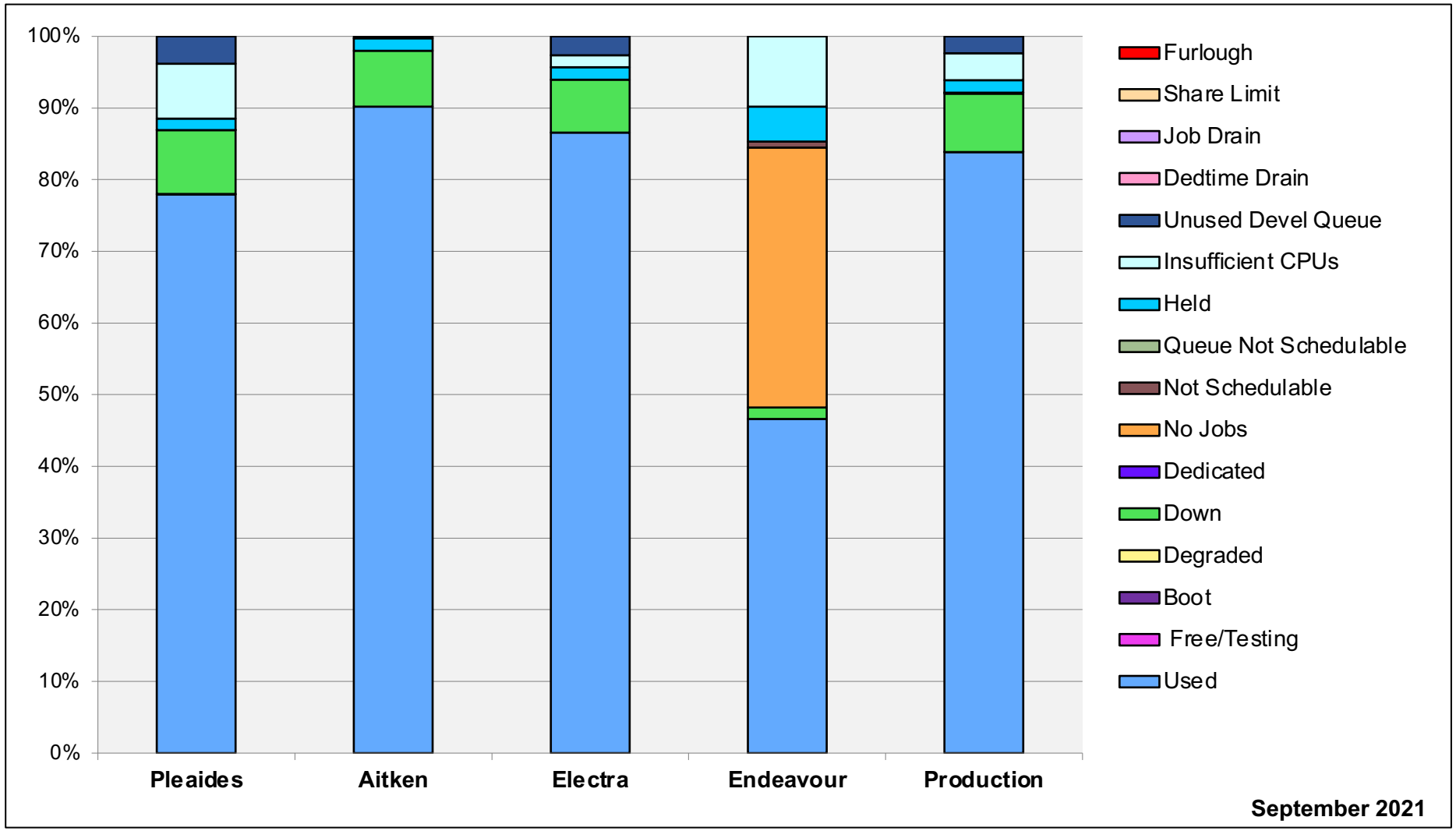
- "**A Uniform Search for Nearby Planetary Companions to Hot Jupiters in TESS Data Reveals Hot Jupiters are Still Lonely**," B. Hord, et al., arXiv:2109.08790 [astro-ph.EP], September 18, 2021. *
  https://arxiv.org/abs/2109.08790
- "**TOI-1296b and TOI-1298b Observed with TESS and SOPHIE: Two Hot Saturn-mass Exoplanets with Different Densities around Metal-rich Stars**," C. Moutou, et al., arXiv:2109.09252 [astro-ph.EP], September 20, 2021. *
  https://arxiv.org/abs/2109.09252
- "**TOI-1201 b: A Mini-Neptune Transiting a Bright and Moderately Young M Dwarf**," D. Kossakowski, et al., arXiv:2109.09346 [astro-ph.EP], September 20, 2021. *
  https://arxiv.org/abs/2109.09346
- "**Impact of Foreshock Transients on the Flank Magnetopause and Magnetosphere and the Ionosphere**," C.-P. Wang, et al., Frontiers in Astronomy and Space Sciences, September 21, 2021. *
  https://www.frontiersin.org/articles/10.3389/fspas.2021.751244/full
- "**Coastal Setting Determines Tidal Marsh Sustainability with Accelerating Sea-Level Rise**," K. Nunez, et al., Ocean & Coastal Management, vol. 214, September 23, 2021. *
  https://www.sciencedirect.com/science/article/abs/pii/S0964569121003811

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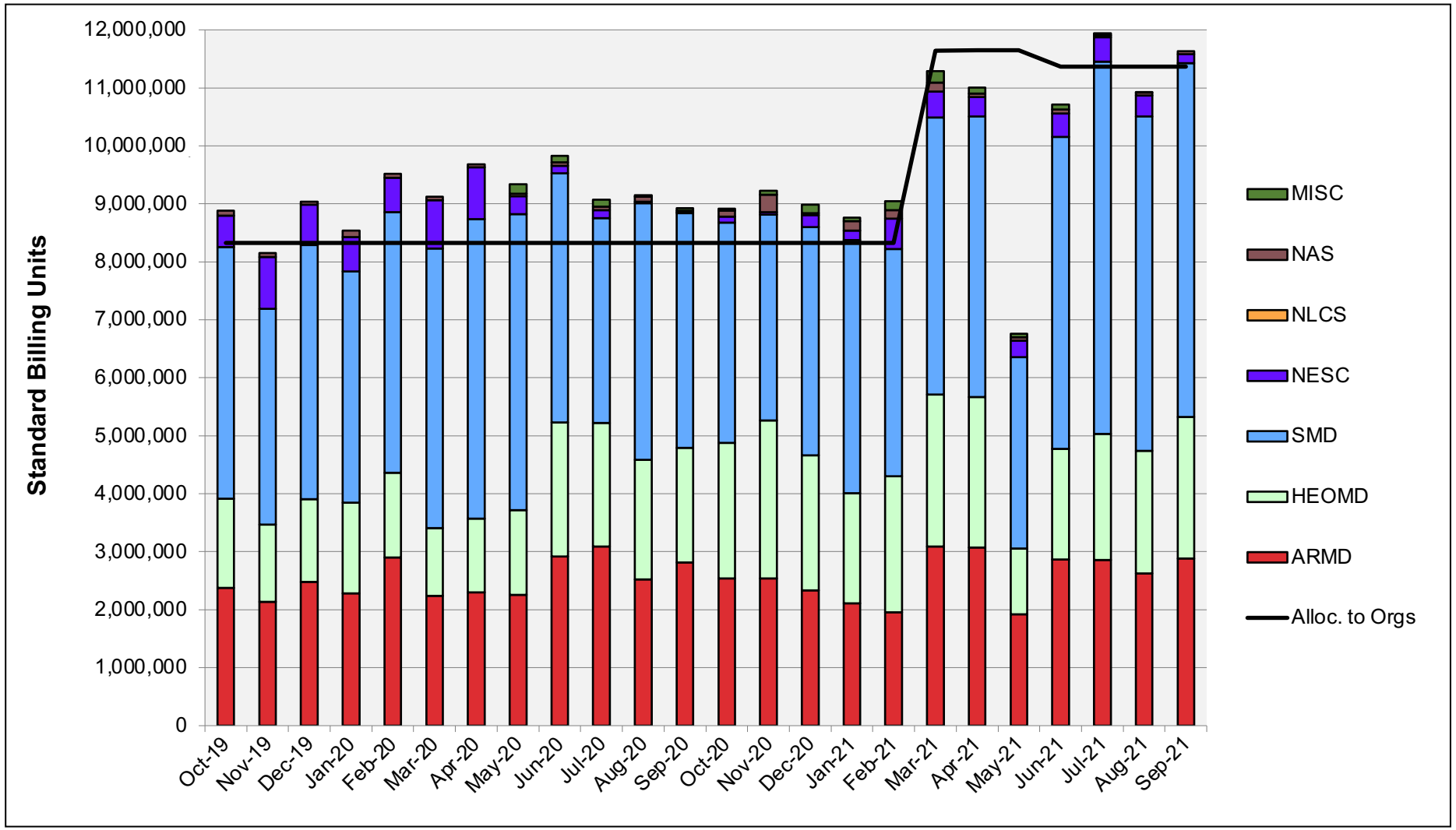
News and Events

- **NASA's First Lunar Rover will Scour the Moon's South Pole for Water in 2023**, *Engadget,* September 3, 2021—With NASA planning to land the world's first autonomous lunar rover to search for water deposits, scientists are creating 3D road maps for the rover to safely explore the lunar surface using the agency's open-source Stereo Pipeline software tool and the Pleiades supercomputer.
  https://www.engadget.com/nasas-first-lunar-rover-will-scour-the-moons-south-pole-for-water-in-2023-160022034-170003713.html
- **The Rock that Ended the Dinosaurs Was Much More than a Dino Killer**, *The New York Times*, September 13, 2021—In his New York Times interview, NAS user Bill Bottke from the Southwest Research Institute described NASA's Pleiades supercomputer as a "game changer" for his research team, which ran simulations of 130,000 model asteroids evolving over hundreds of millions of years—including the one that may have killed off the dinosaurs.
  https://www.nytimes.com/2021/09/13/science/chicxulub-dinosaur-extinction.html

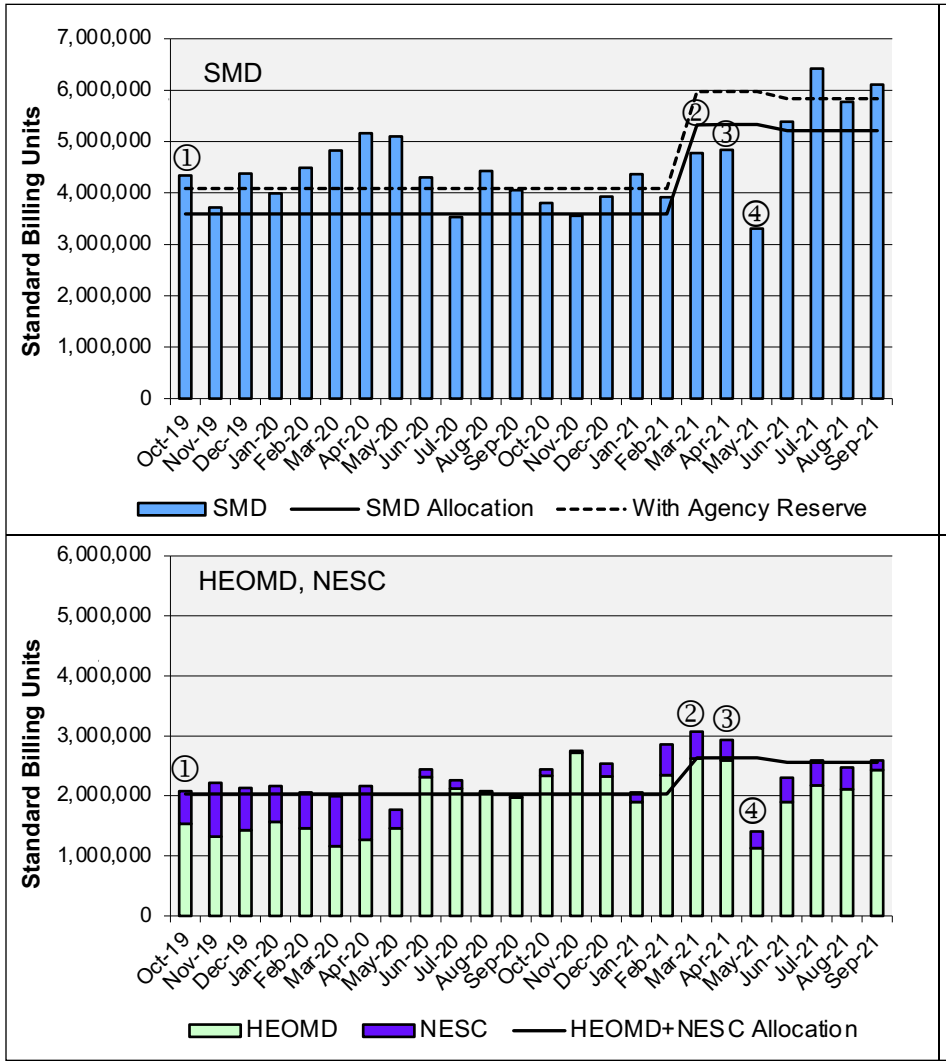
HECC Utilization

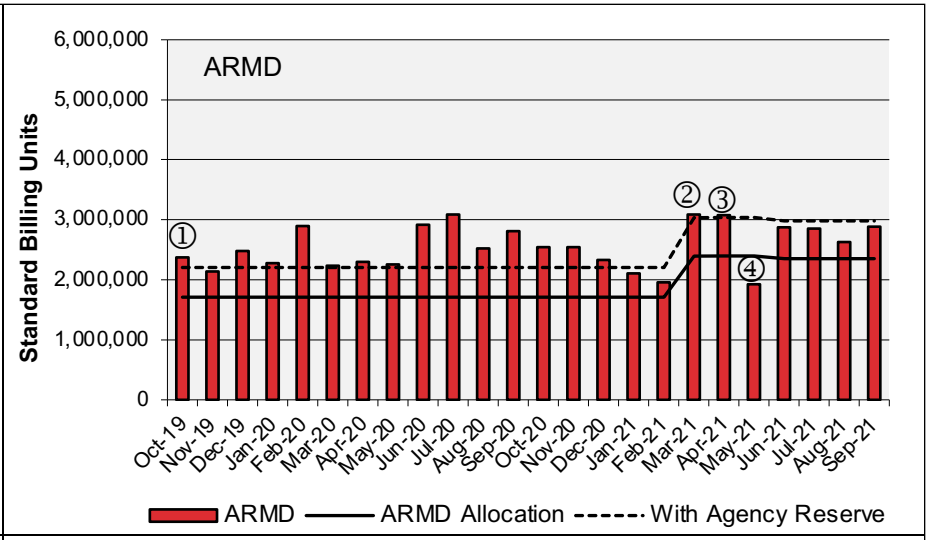


HECC Utilization Normalized to 30-Day Month



HECC Utilization Normalized to 30-Day Month





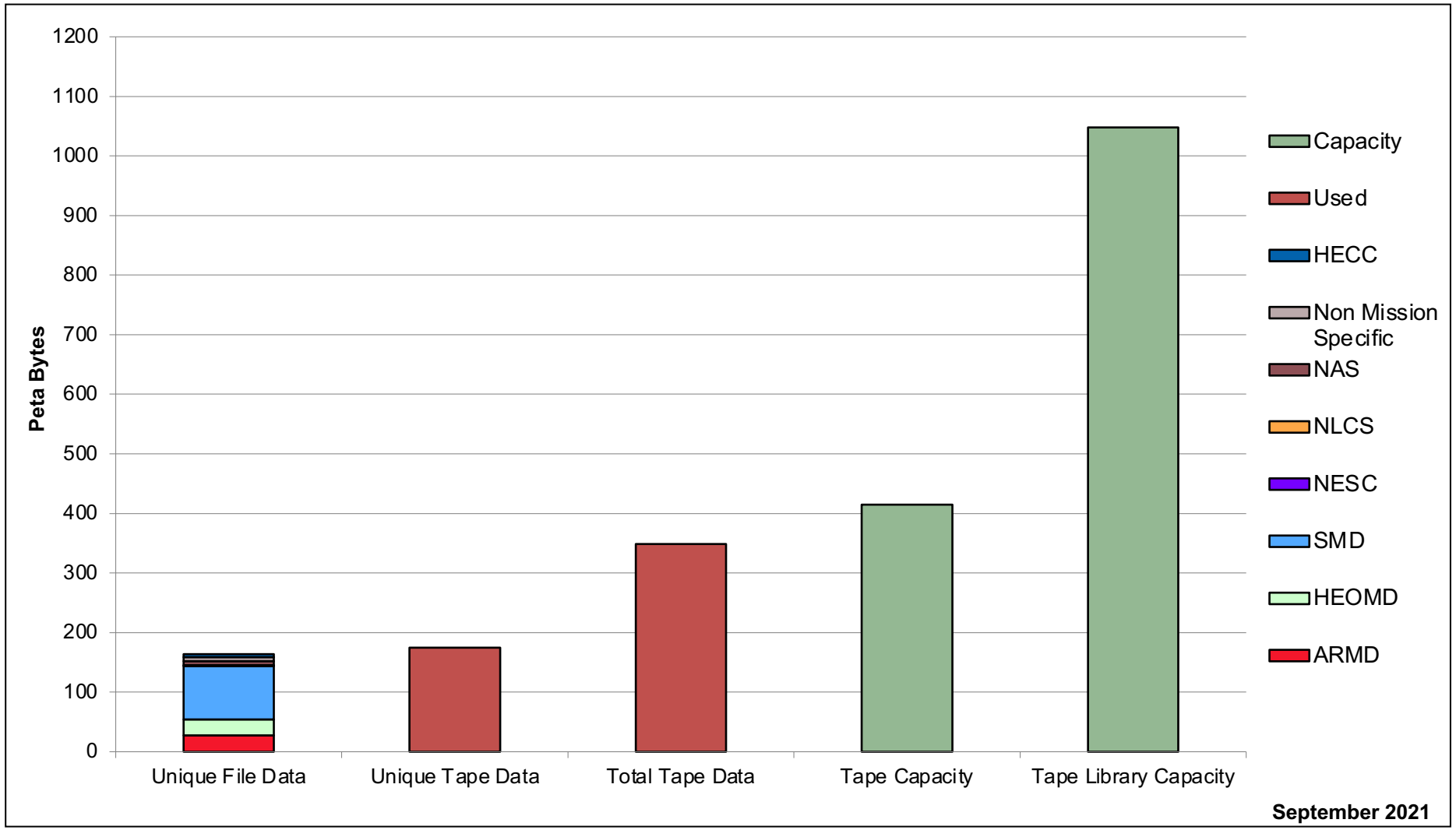
① 4 Cascade Lake E cells introduced into Aitken

② 8 Rome Apollo racks introduced into Aitken

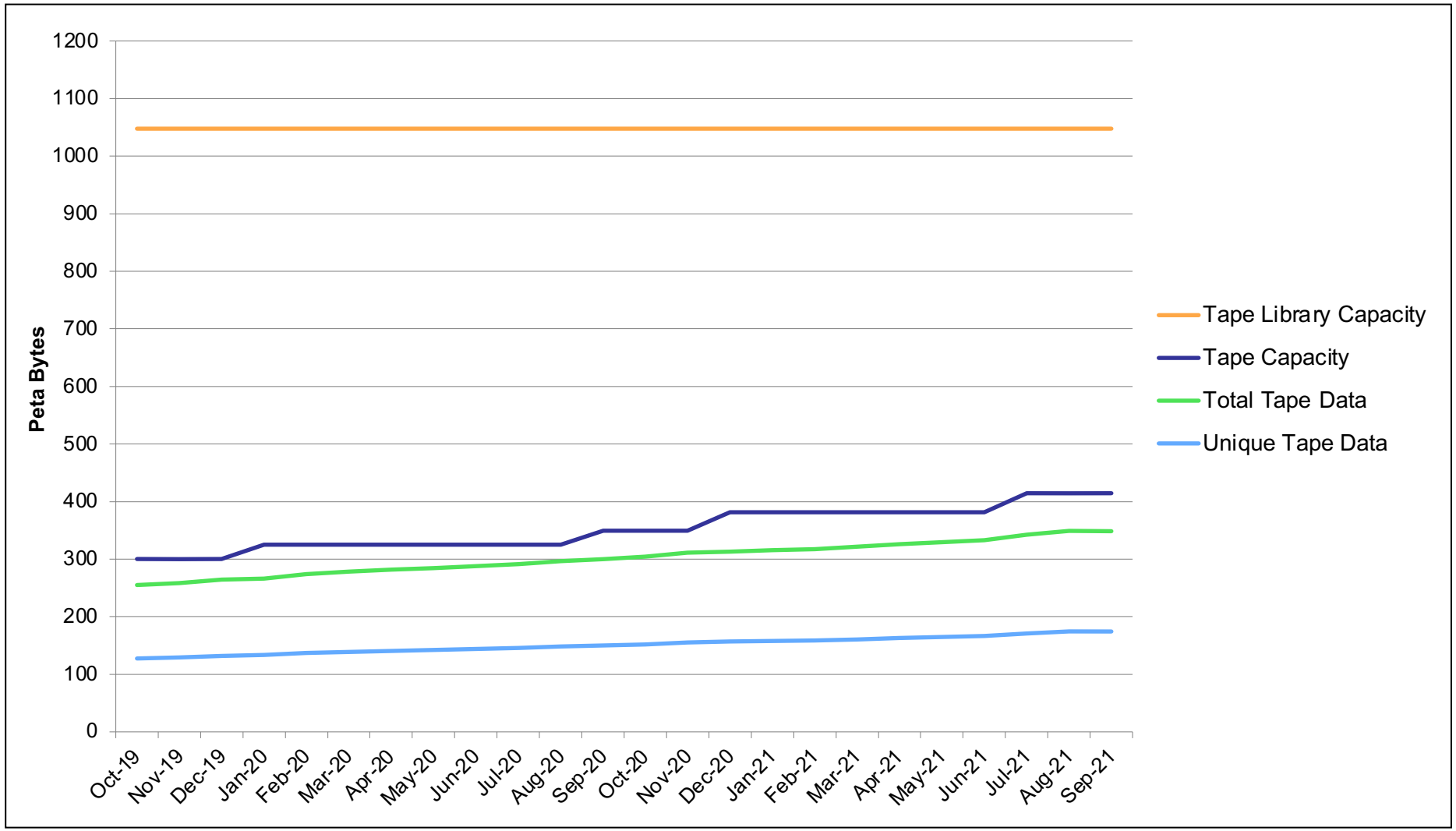
③ Endeavour replaced with new hardware

④ Merope retired, Annual Maintenance

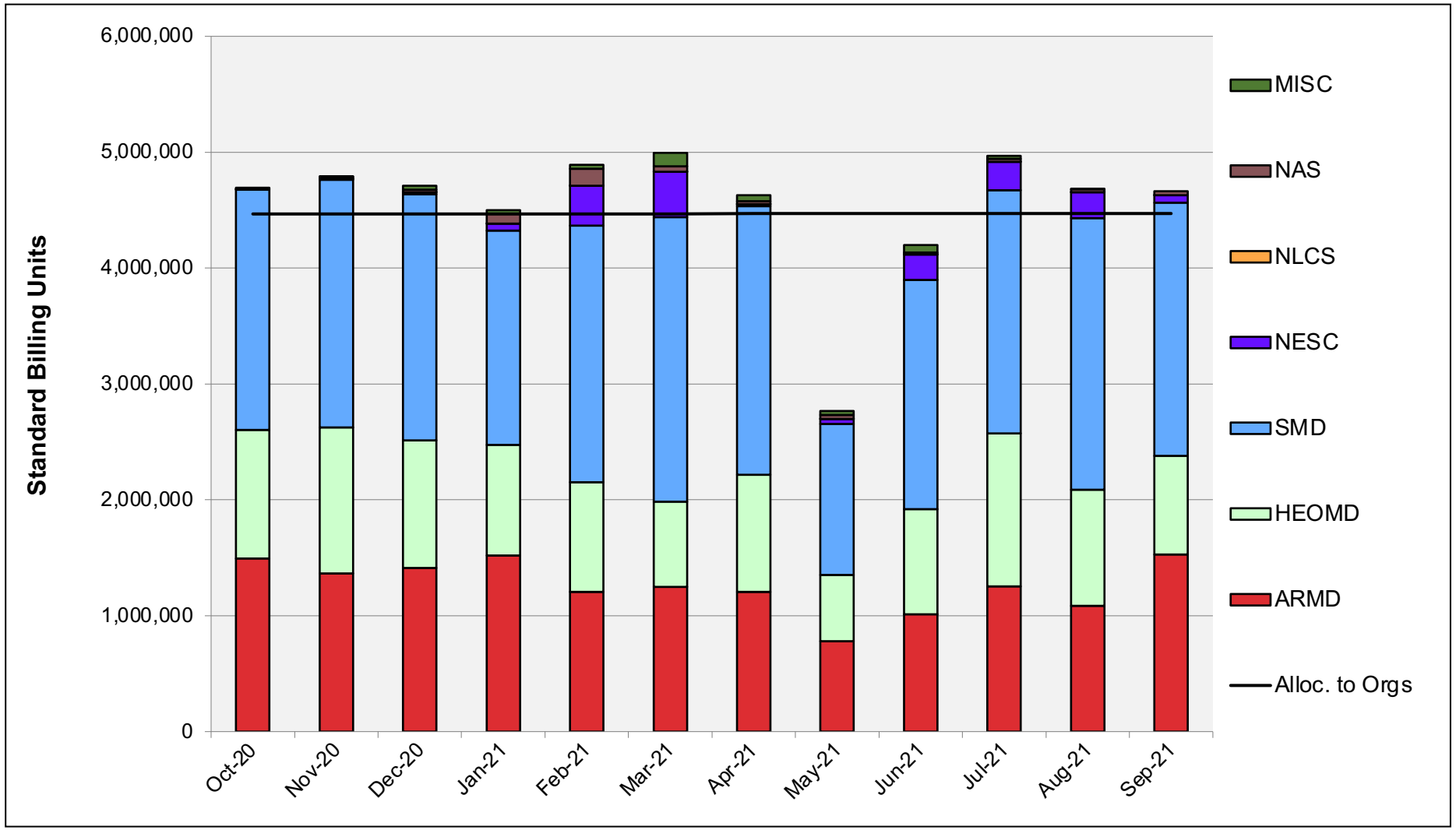
Tape Archive Status



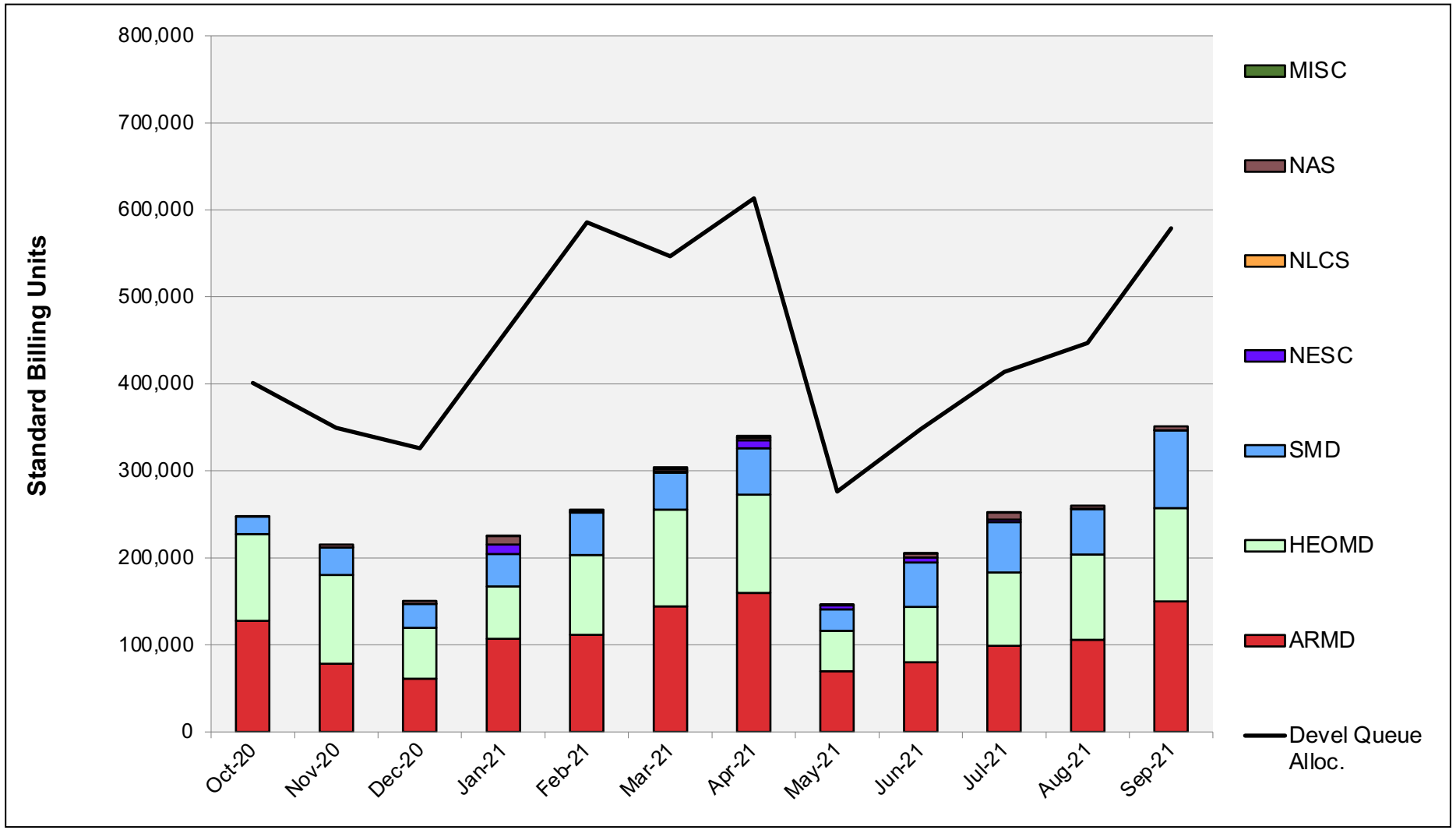
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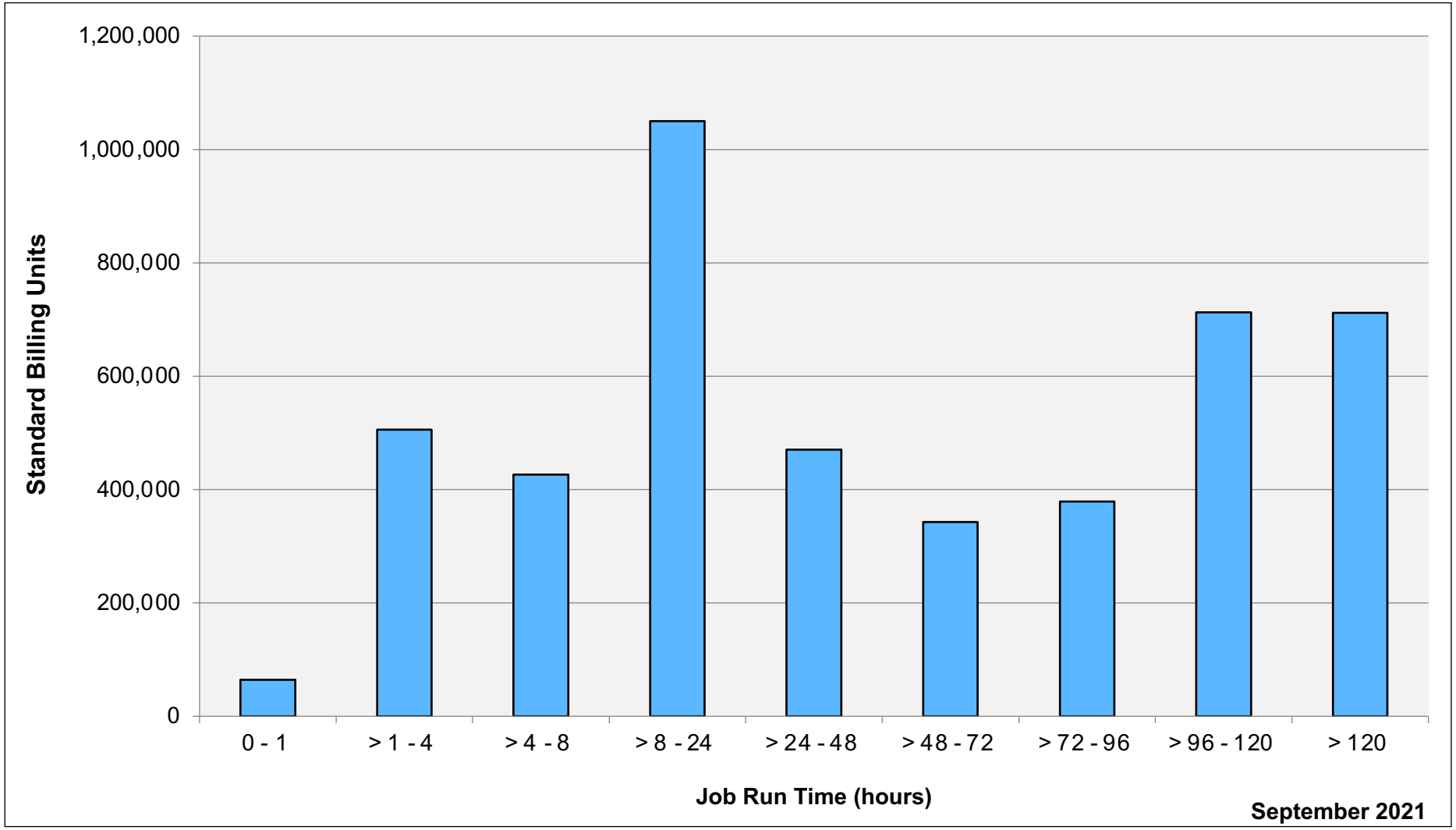
Pleiades: SBUs Reported, Normalized to 30-Day Month



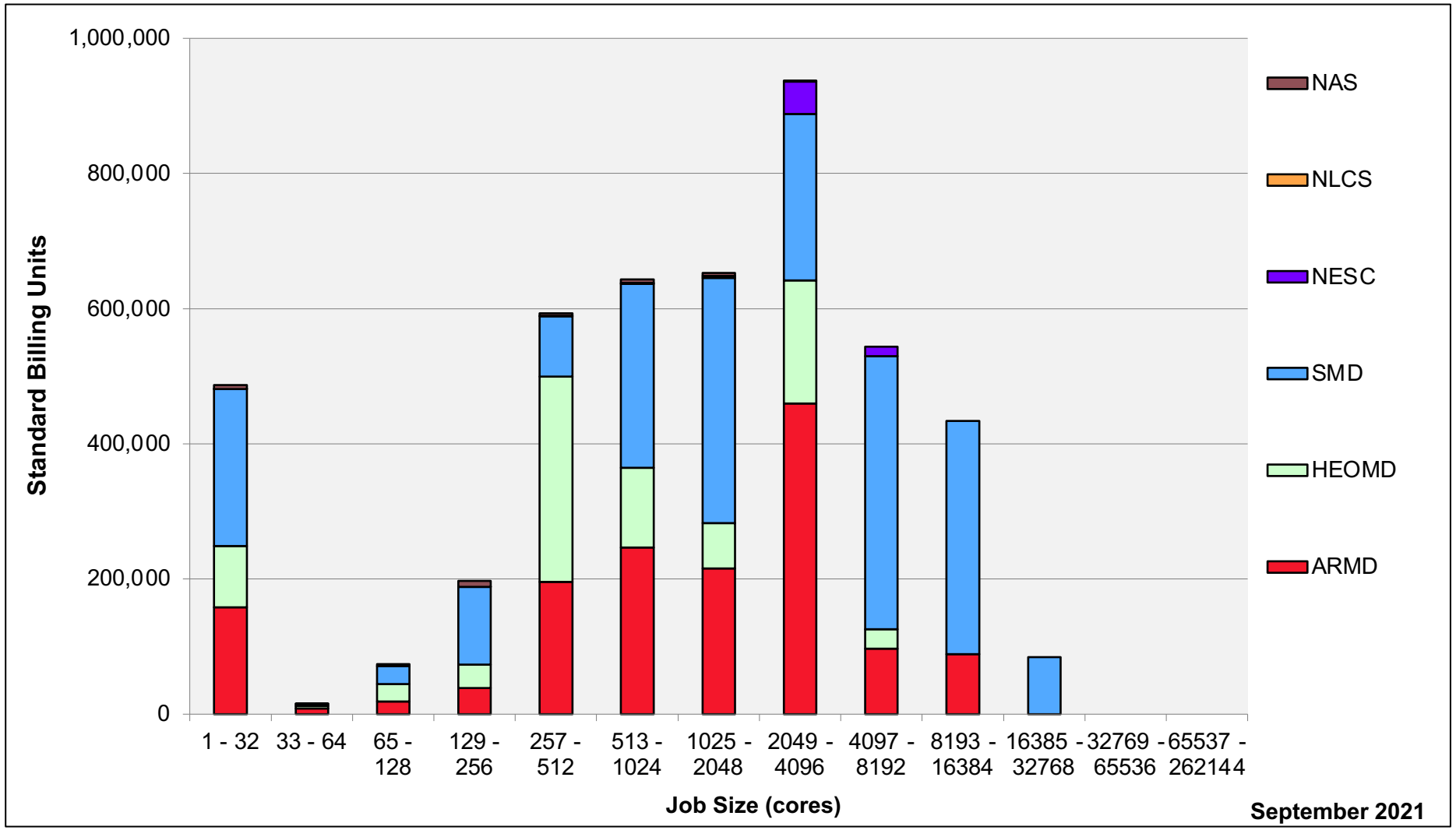
Pleiades: Devel Queue Utilization



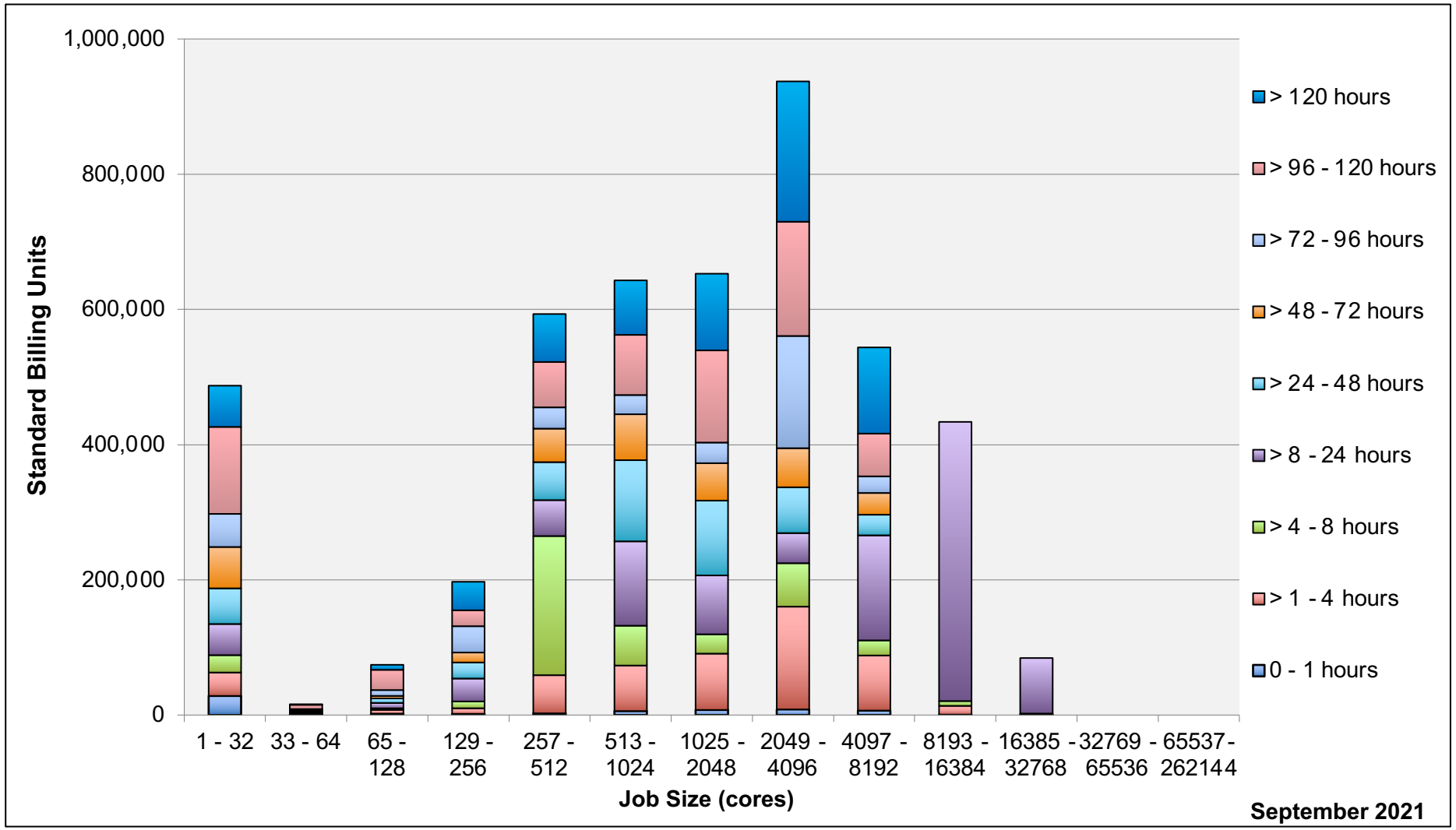
Pleiades: Monthly Utilization by Job Length



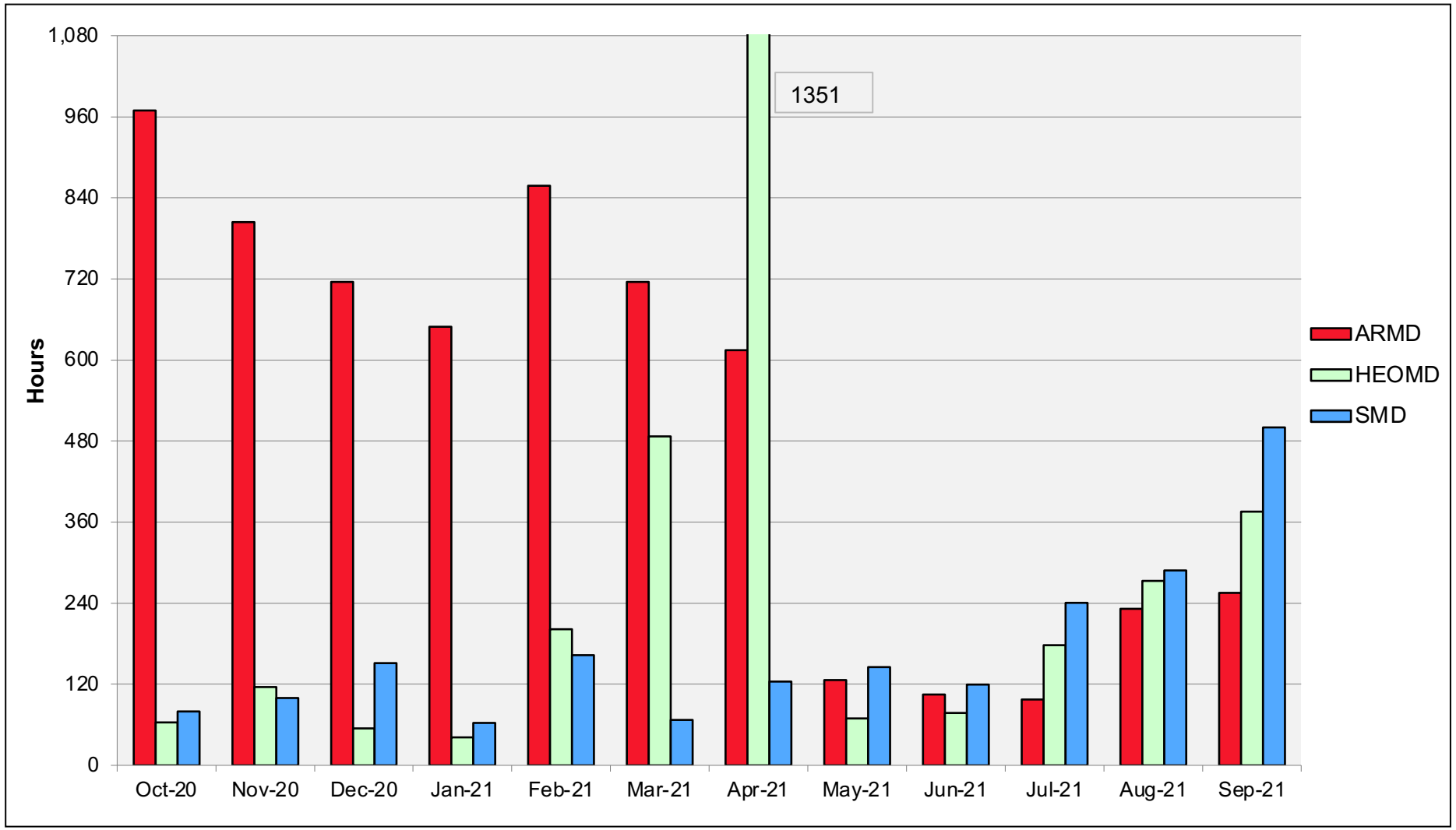
Pleiades: Monthly Utilization by Job Size



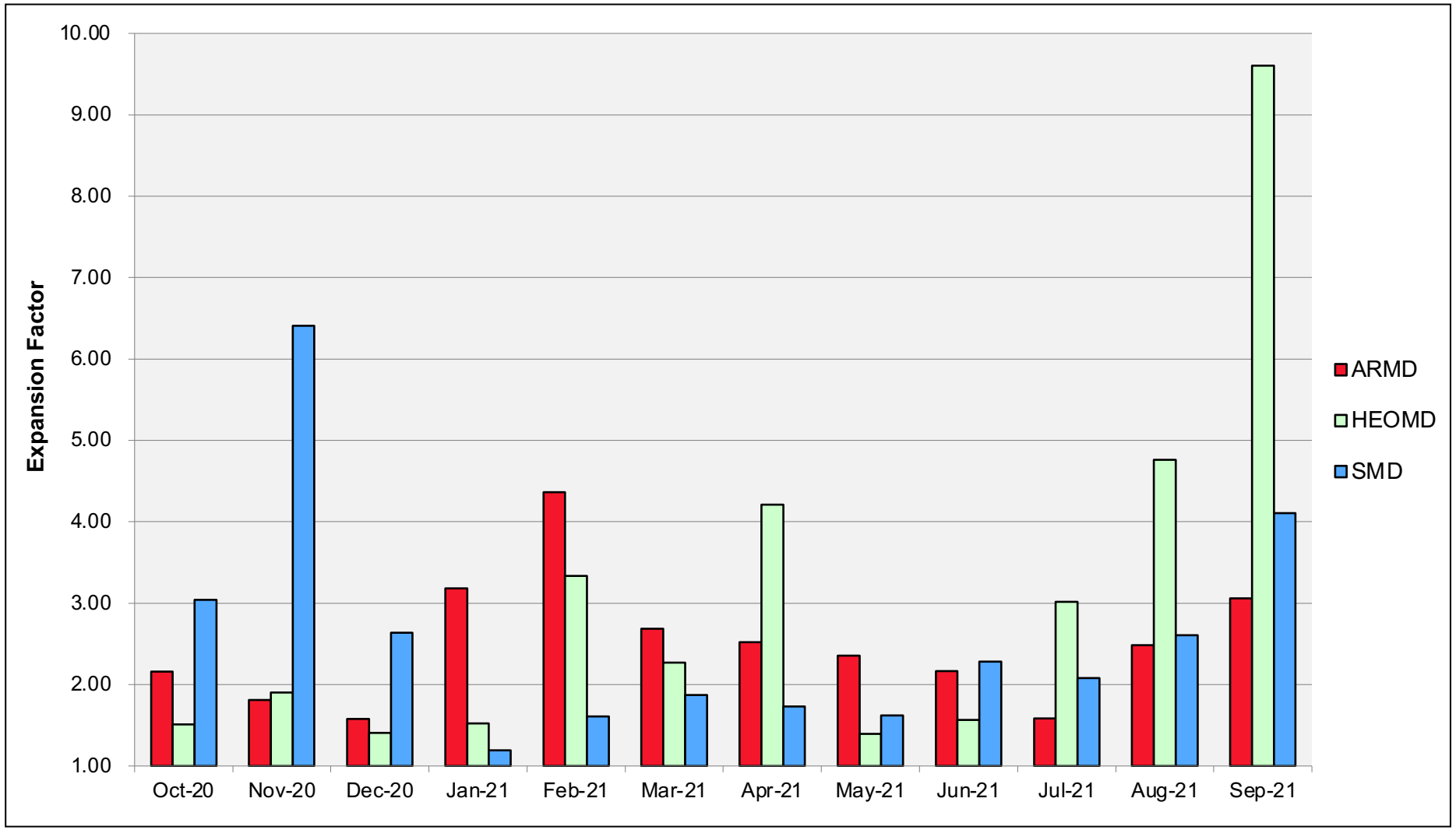
Pleiades: Monthly Utilization by Size and Length



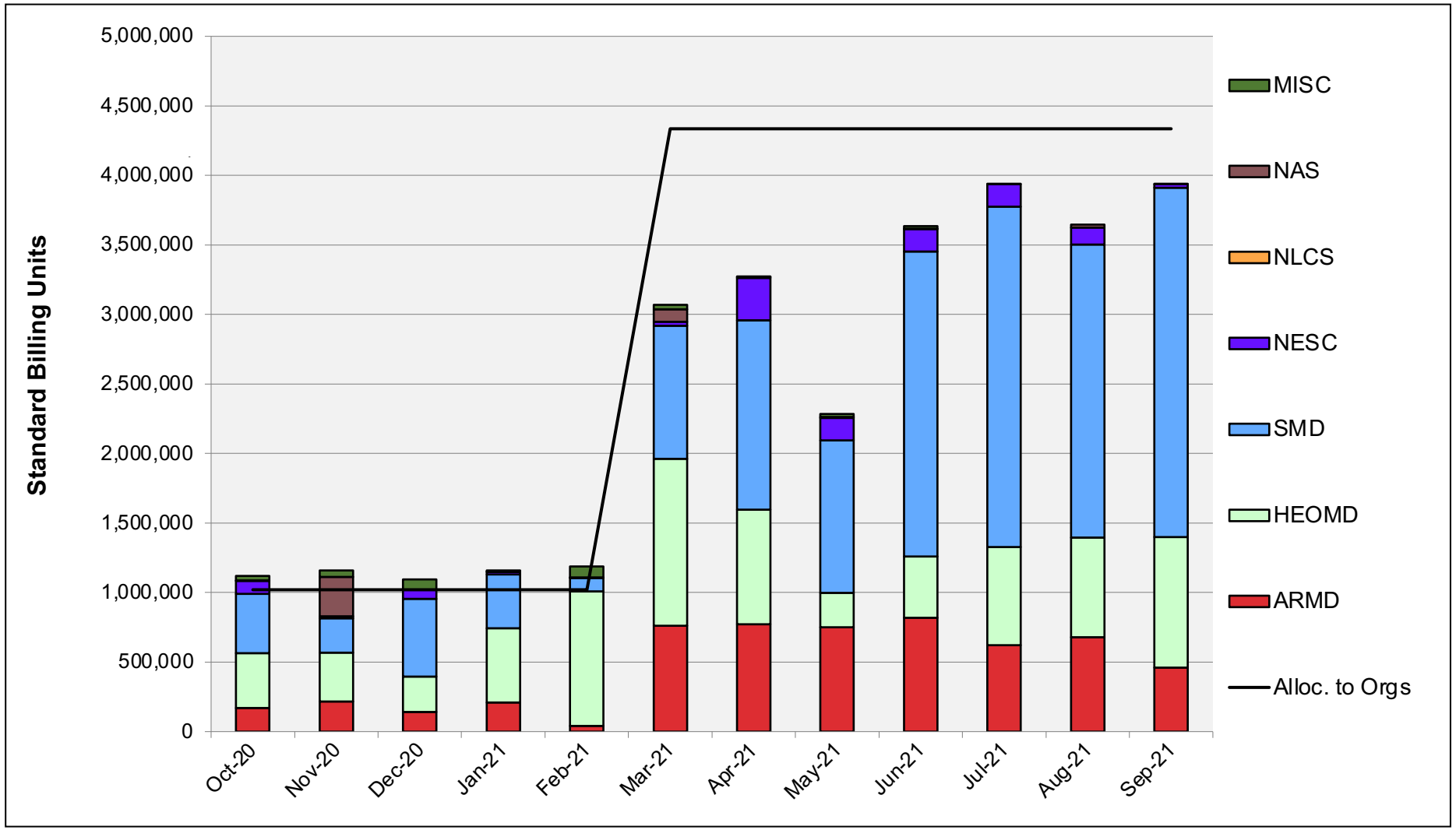
Pleiades: Average Time to Clear All Jobs



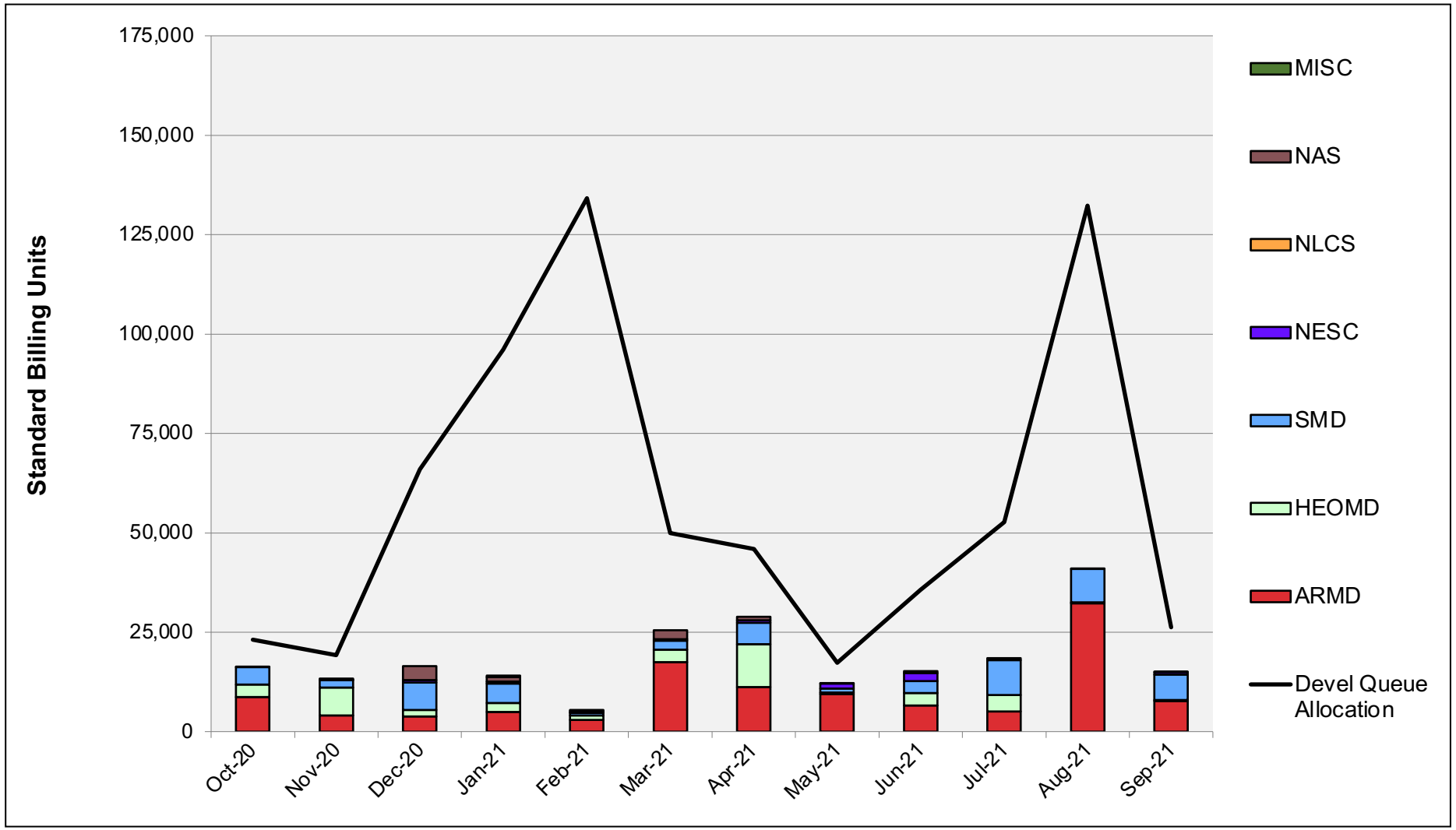
Pleiades: Average Expansion Factor



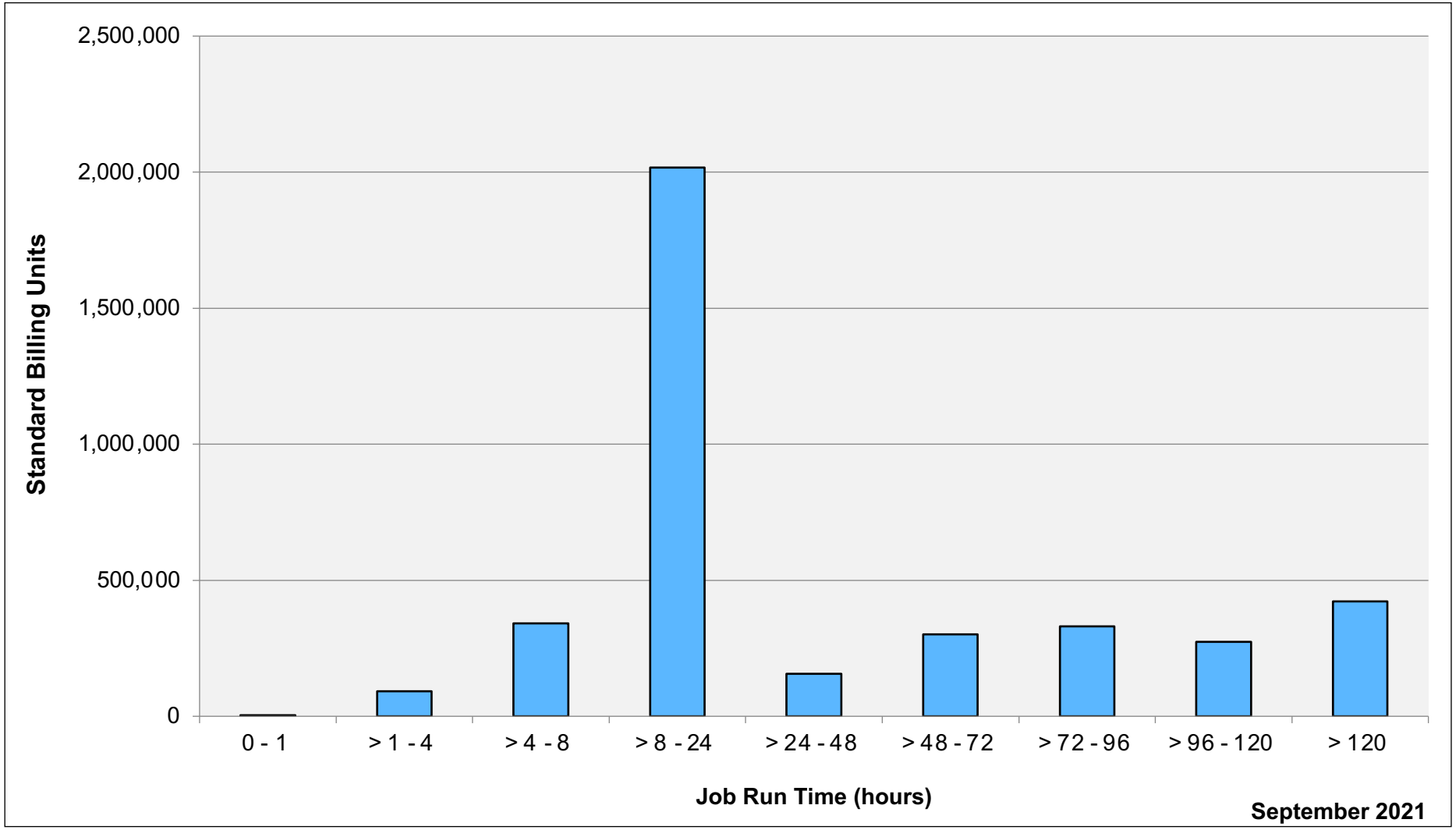
Aitken: SBUs Reported, Normalized to 30-Day Month



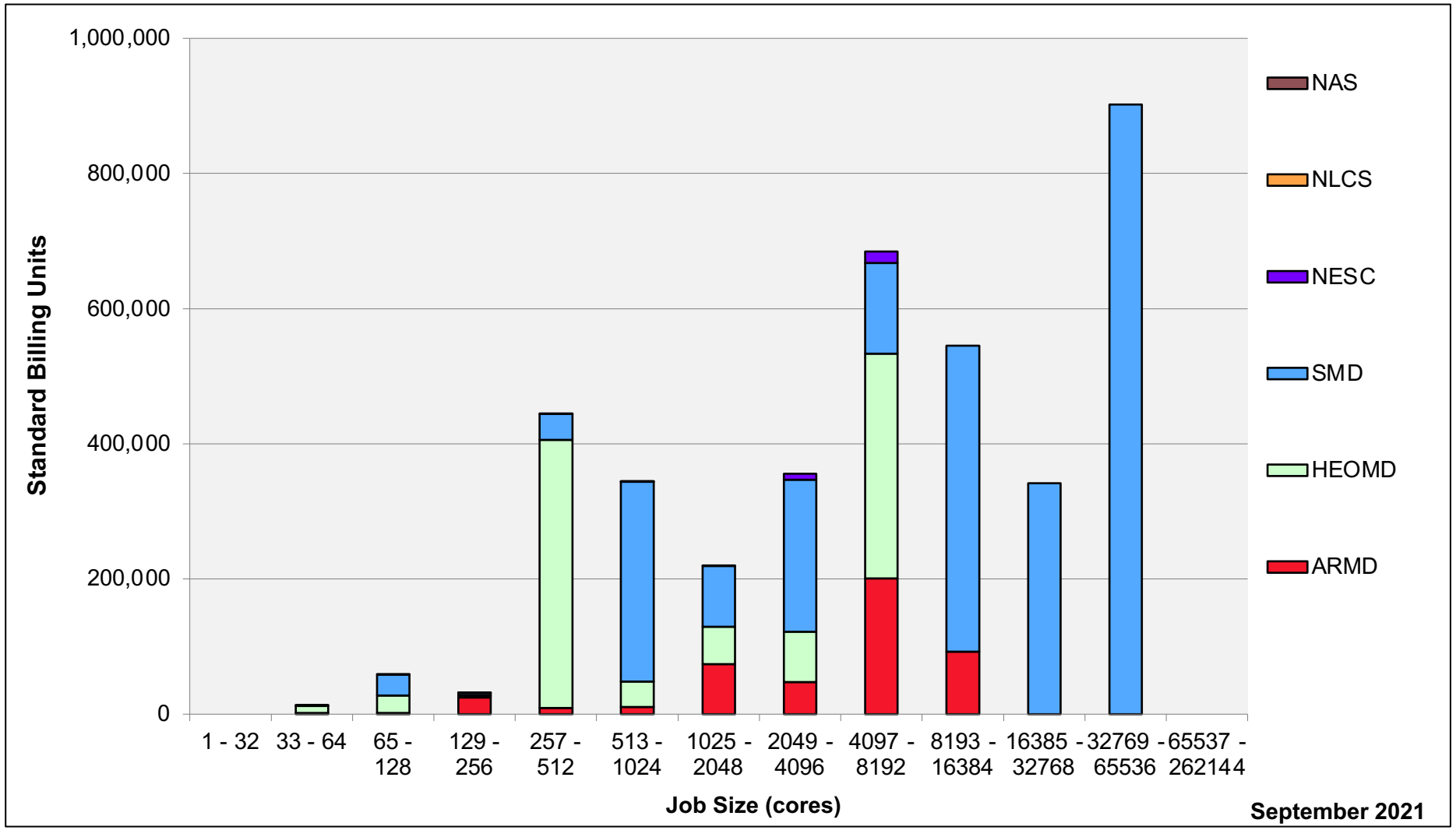
Aitken: Devel Queue Utilization



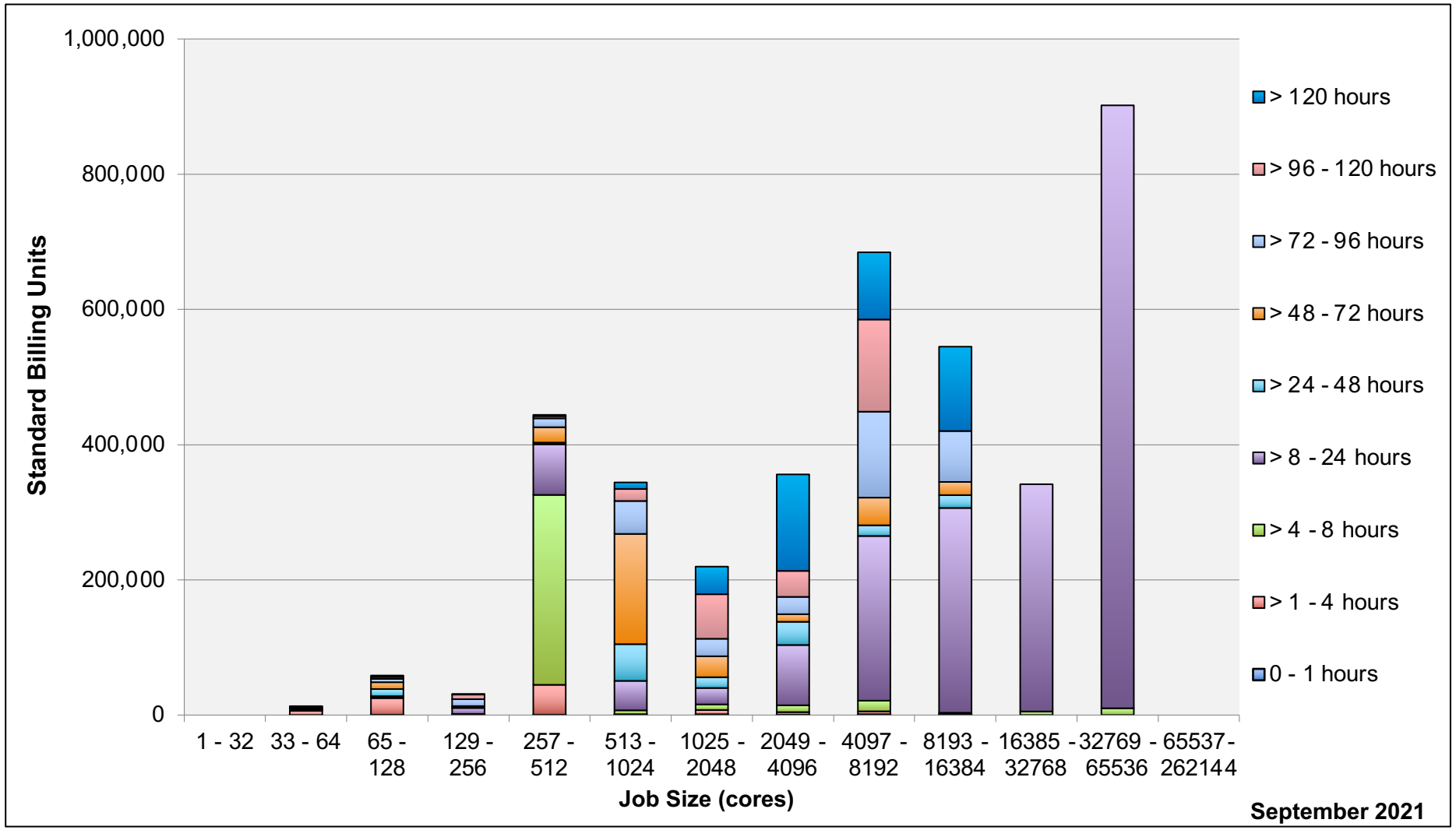
Aitken: Monthly Utilization by Job Length



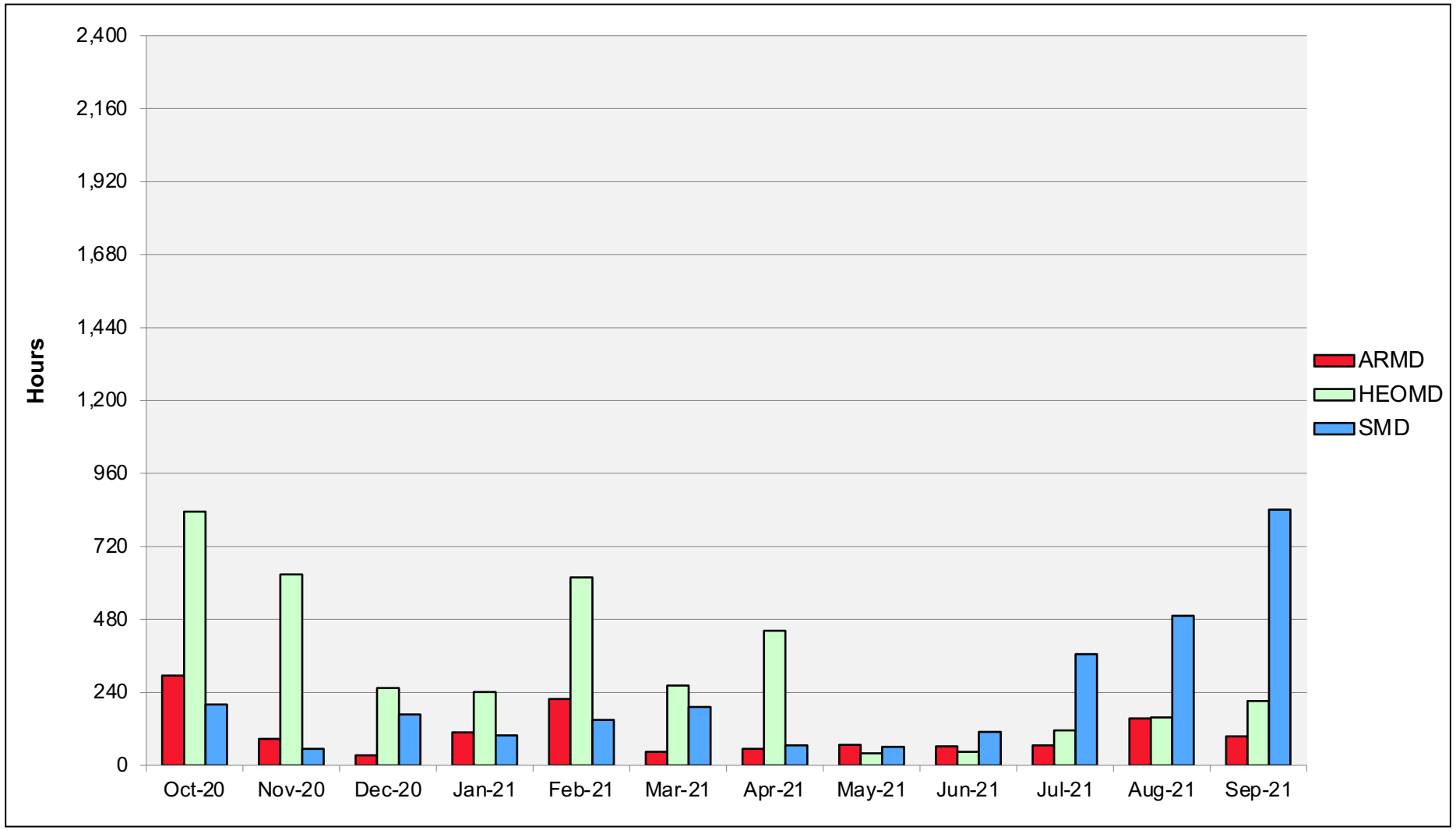
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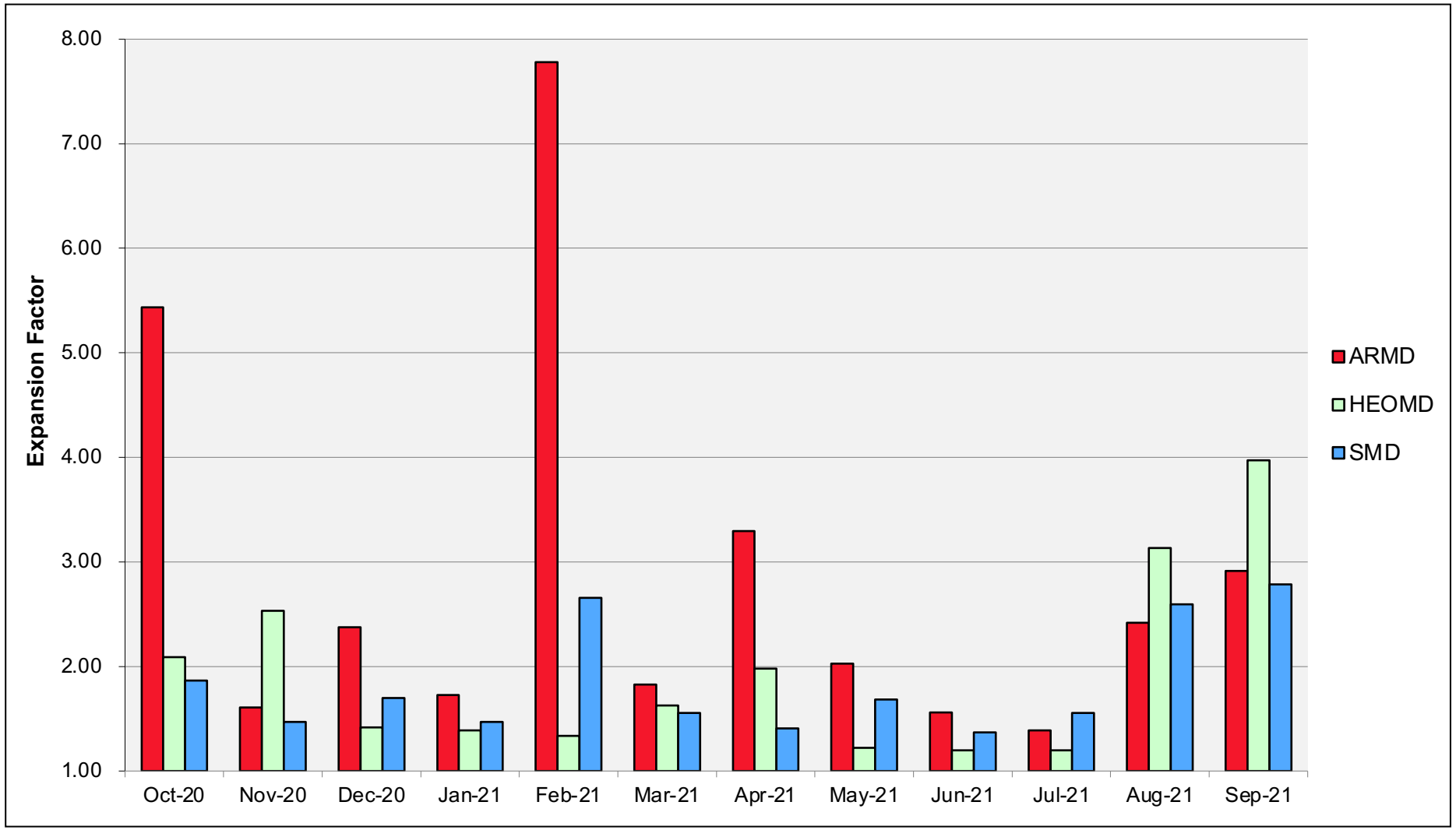
Aitken: Monthly Utilization by Size and Length



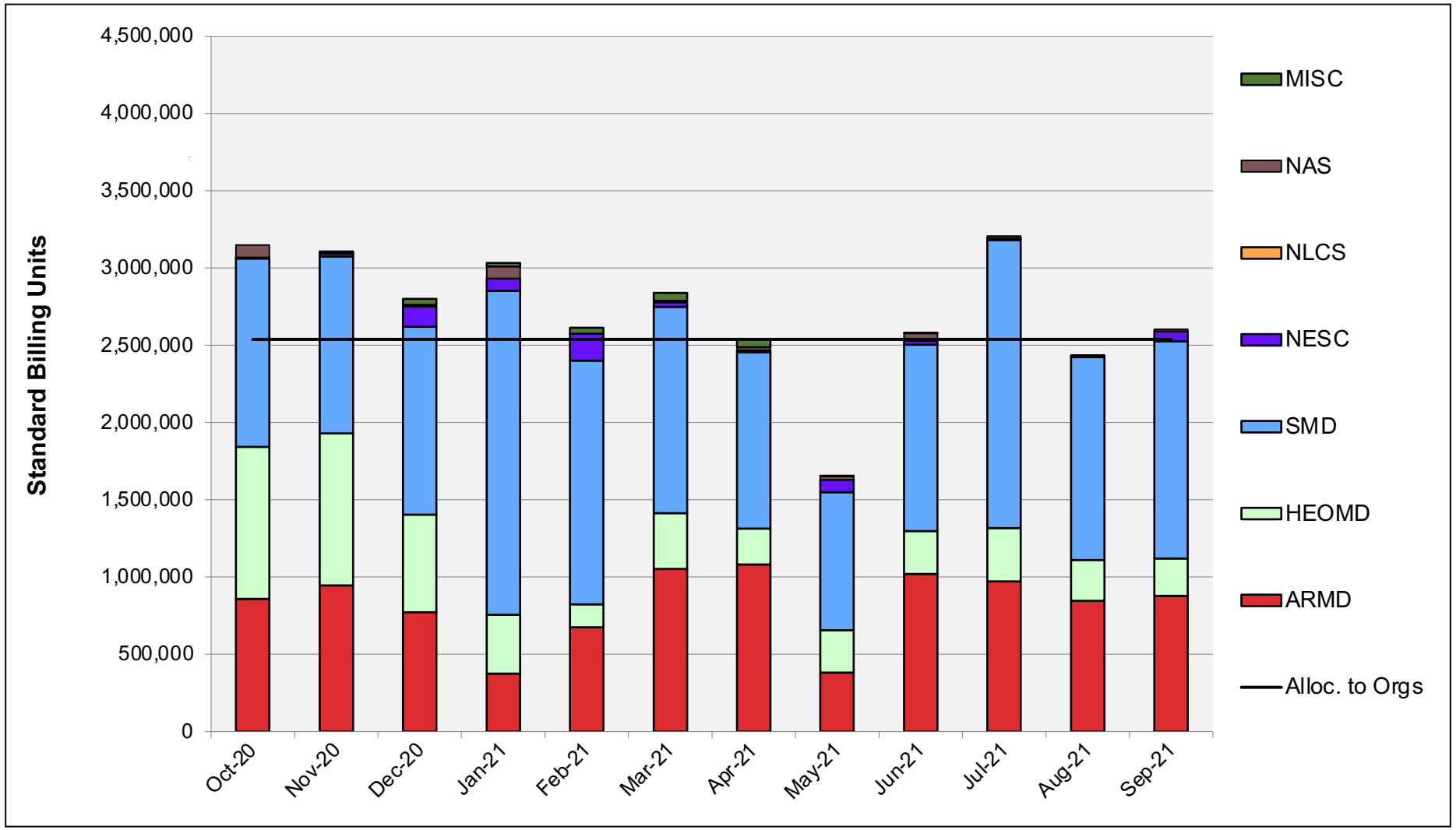
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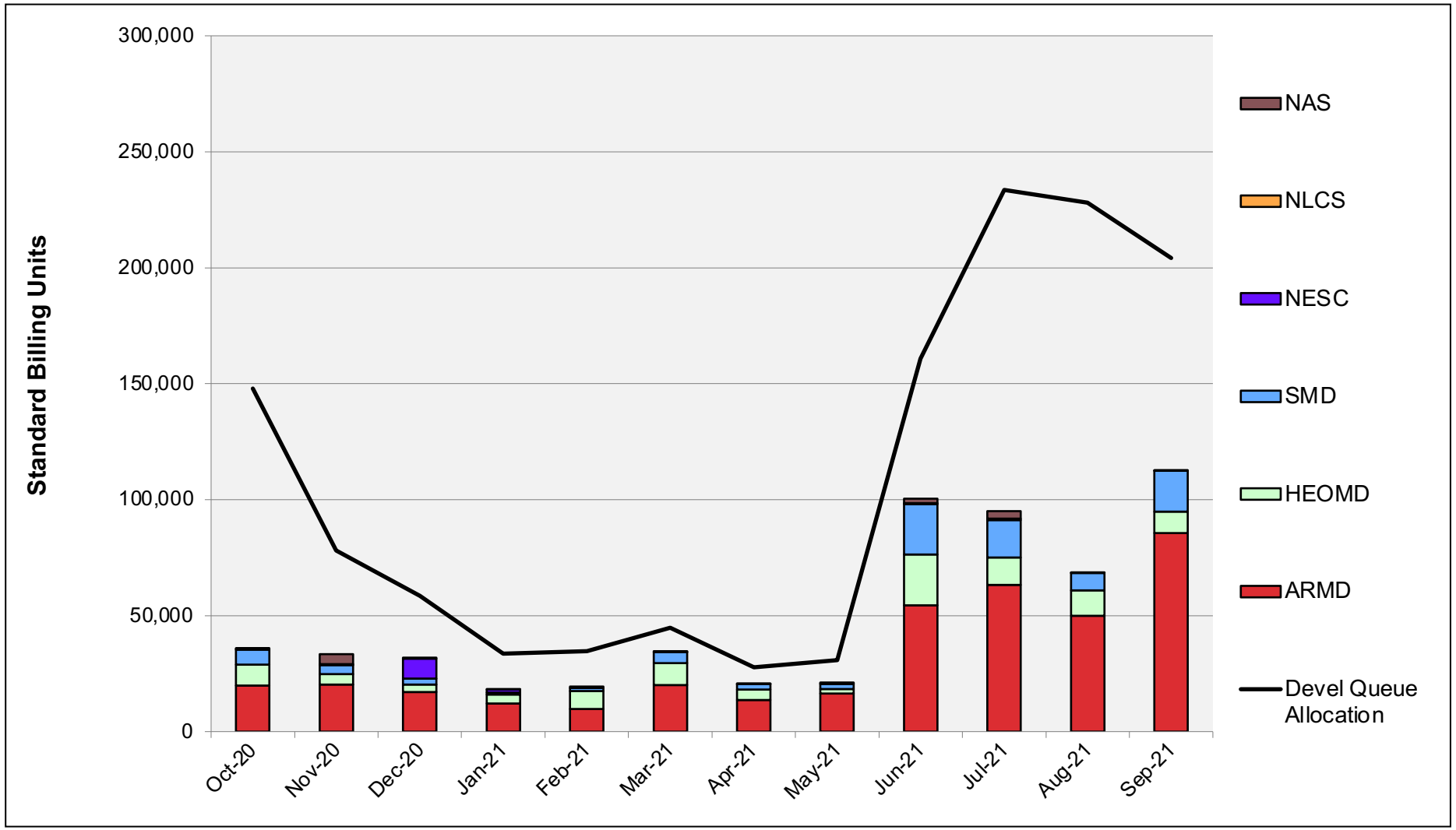
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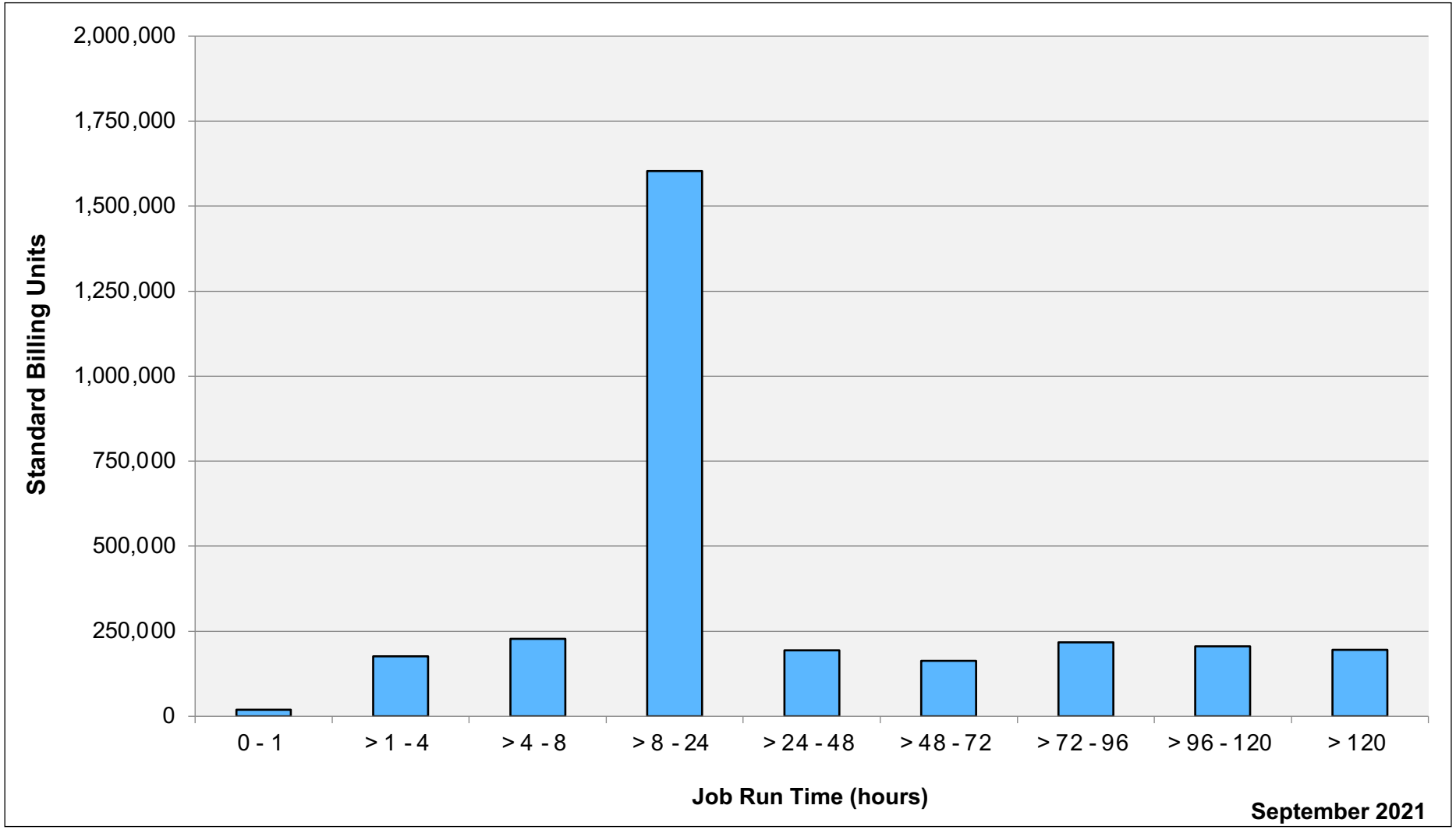
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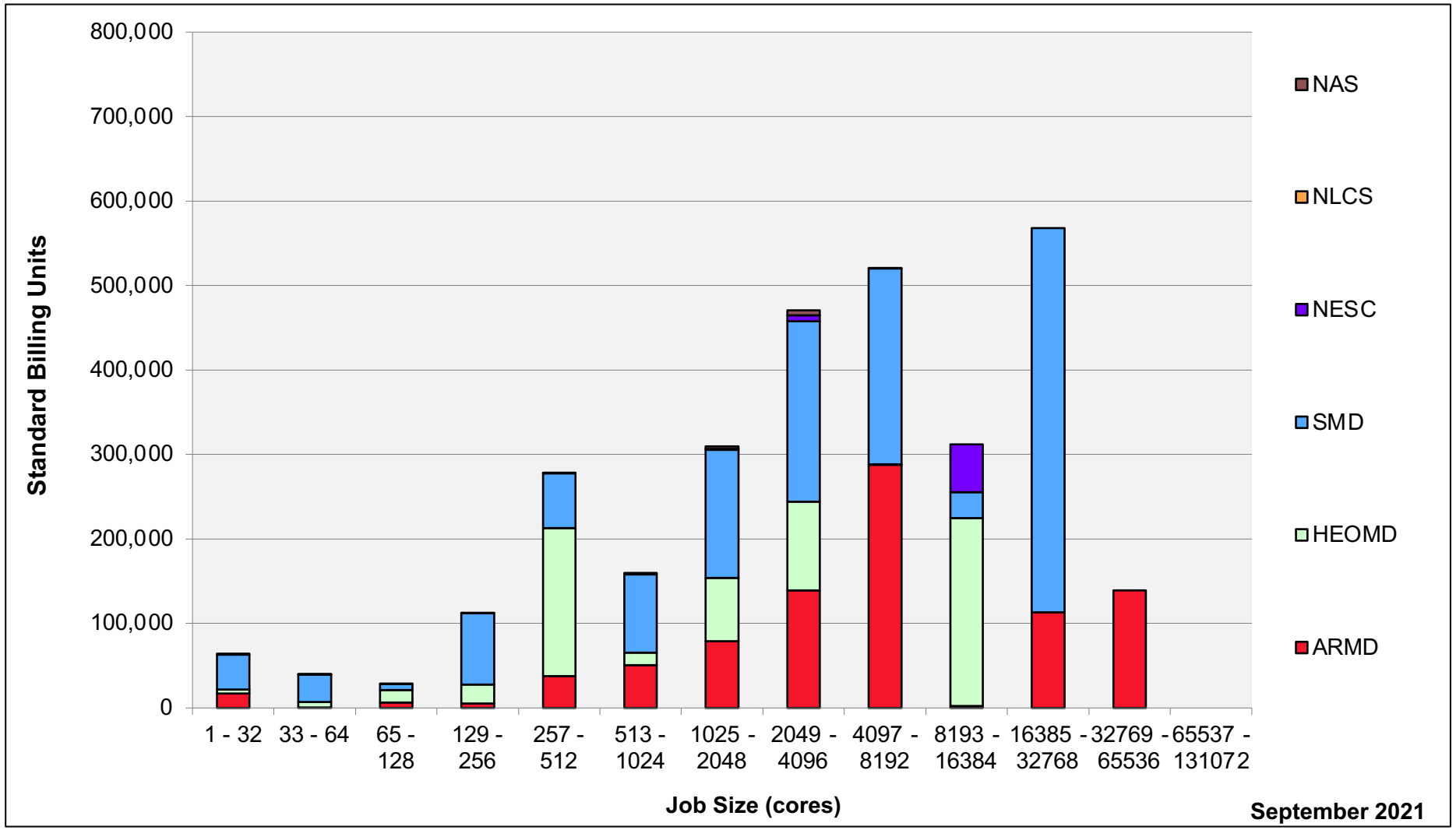
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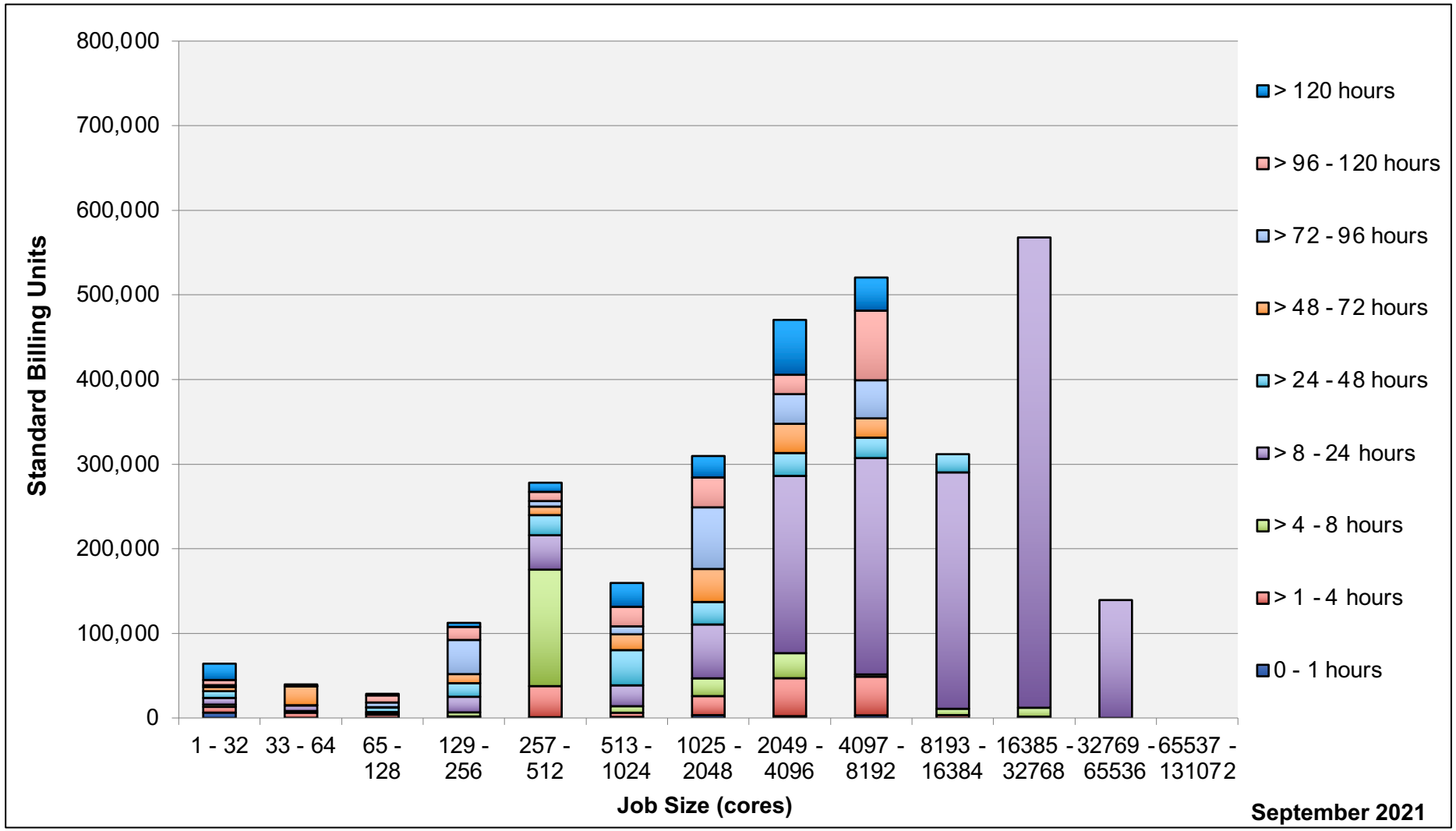
Electra: Monthly Utilization by Job Length



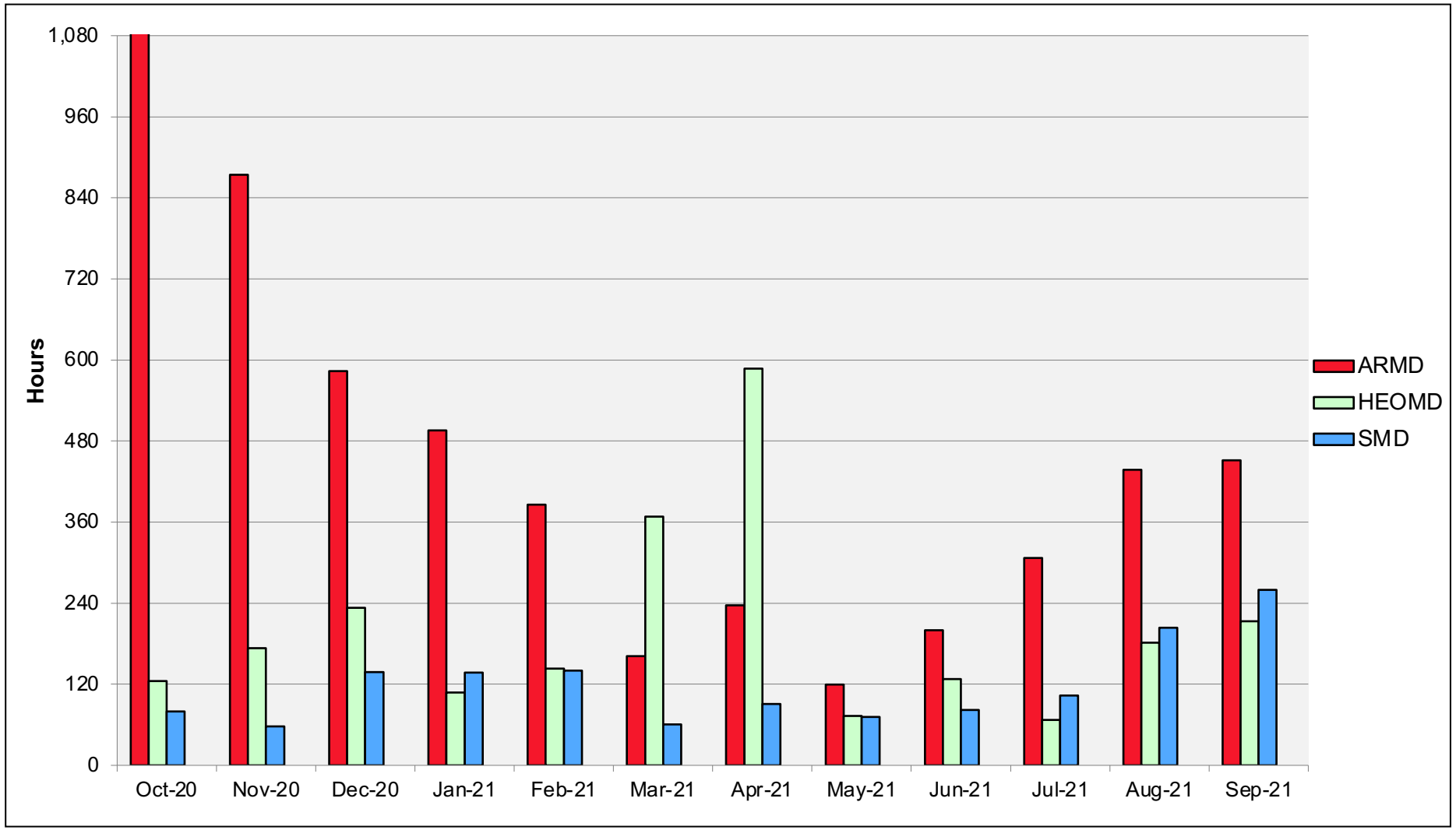
Electra: Monthly Utilization by Job Size



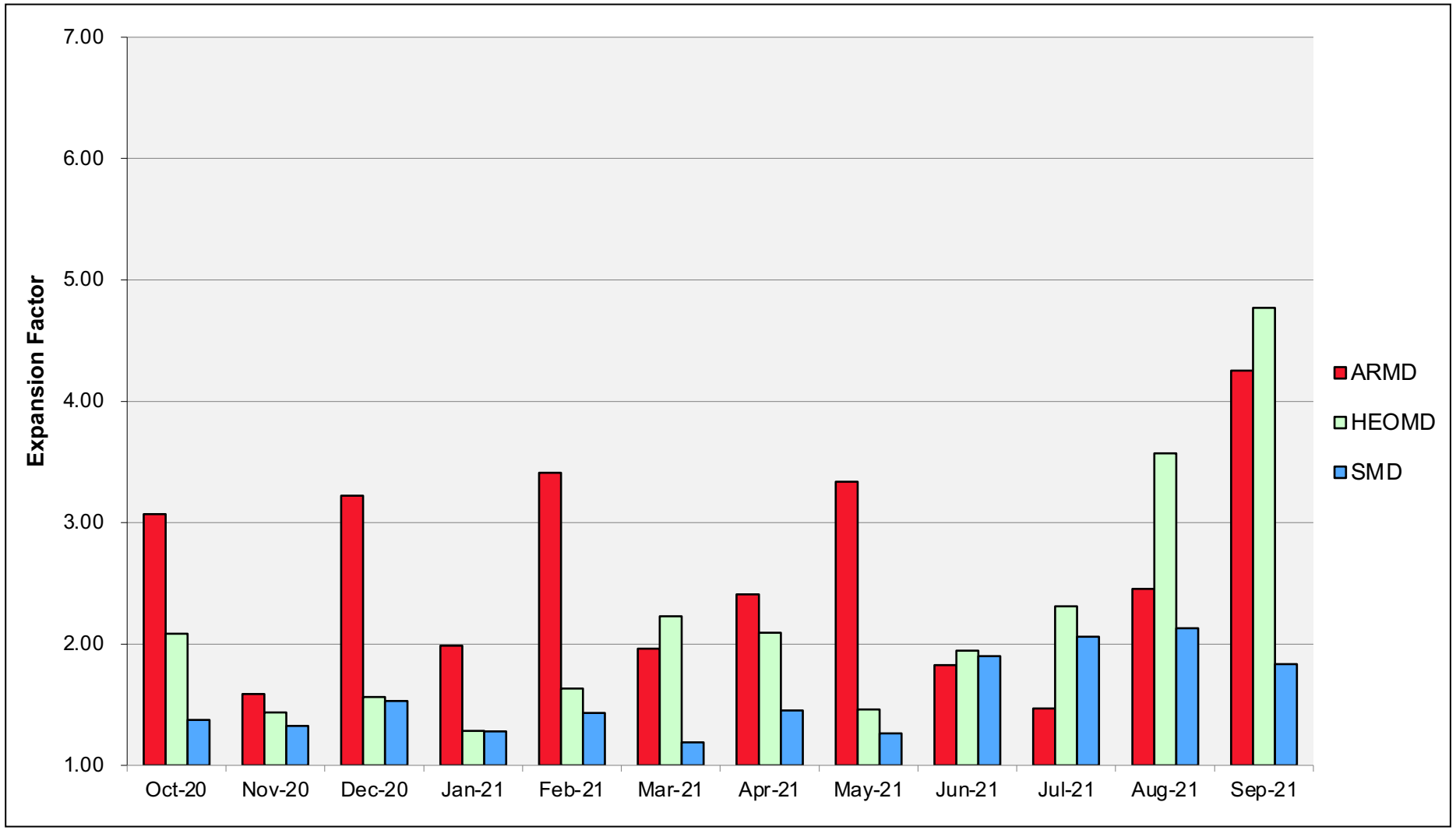
Electra: Monthly Utilization by Size and Length



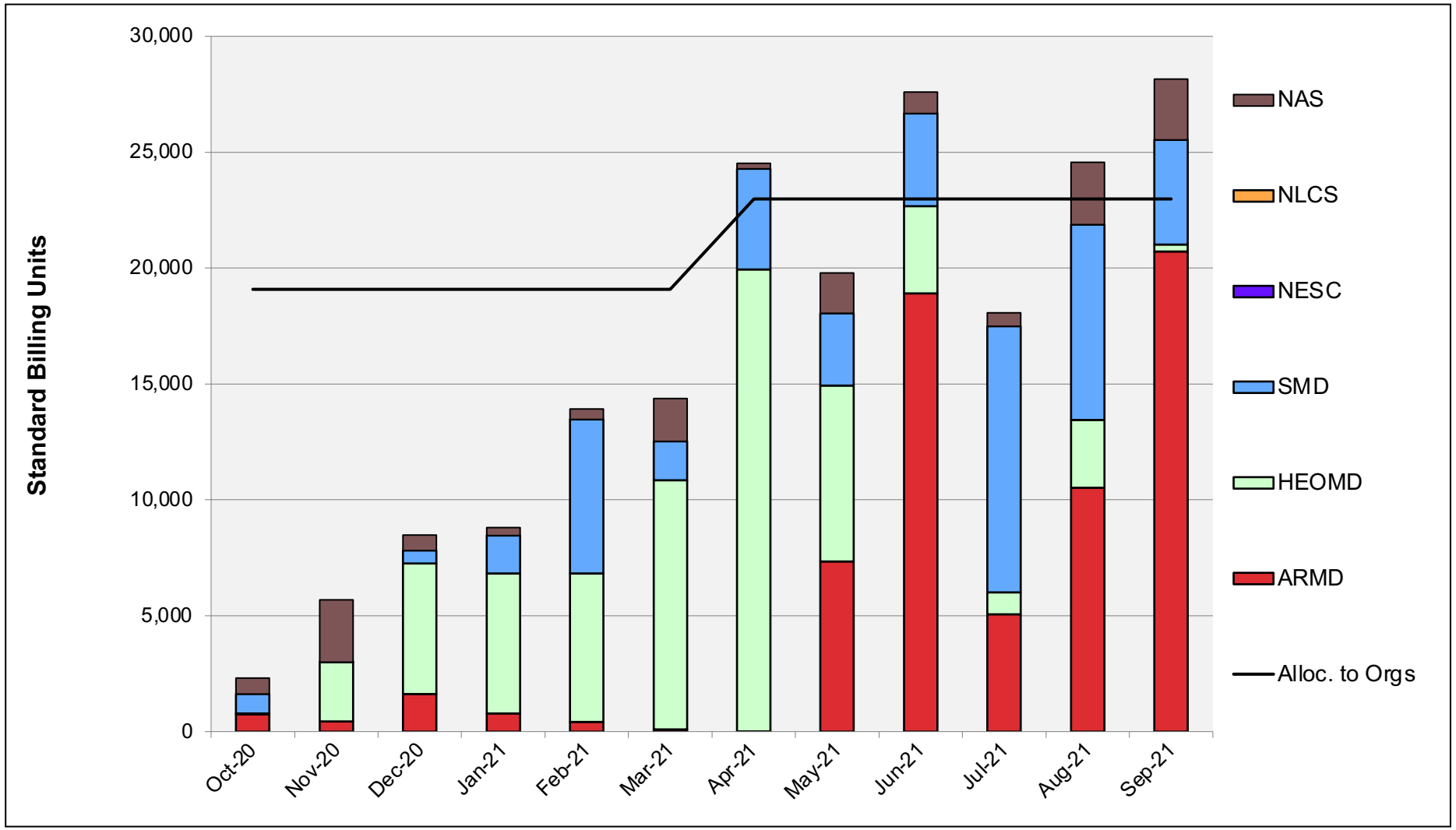
Electra: Average Time to Clear All Jobs



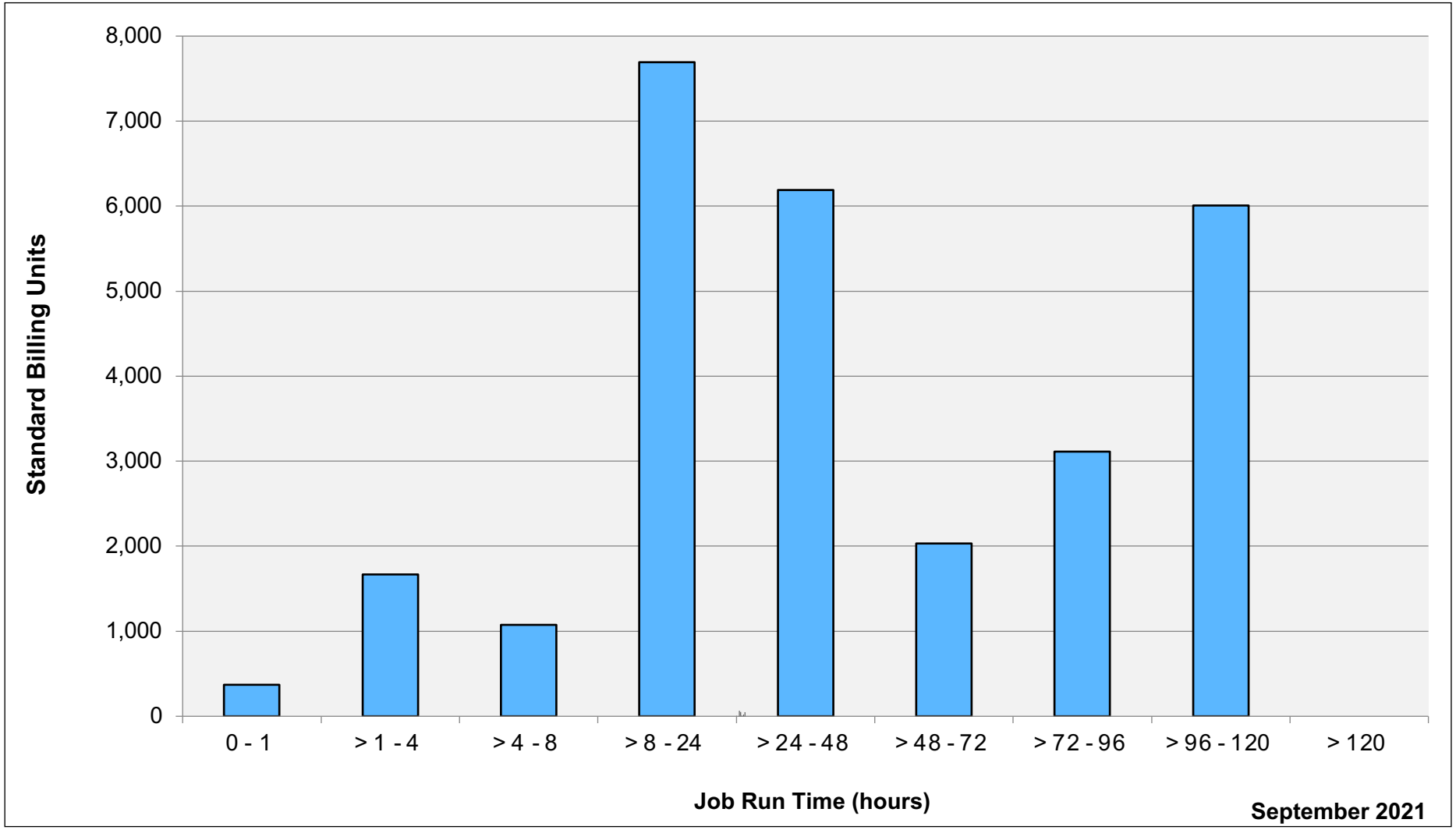
Electra: Average Expansion Factor



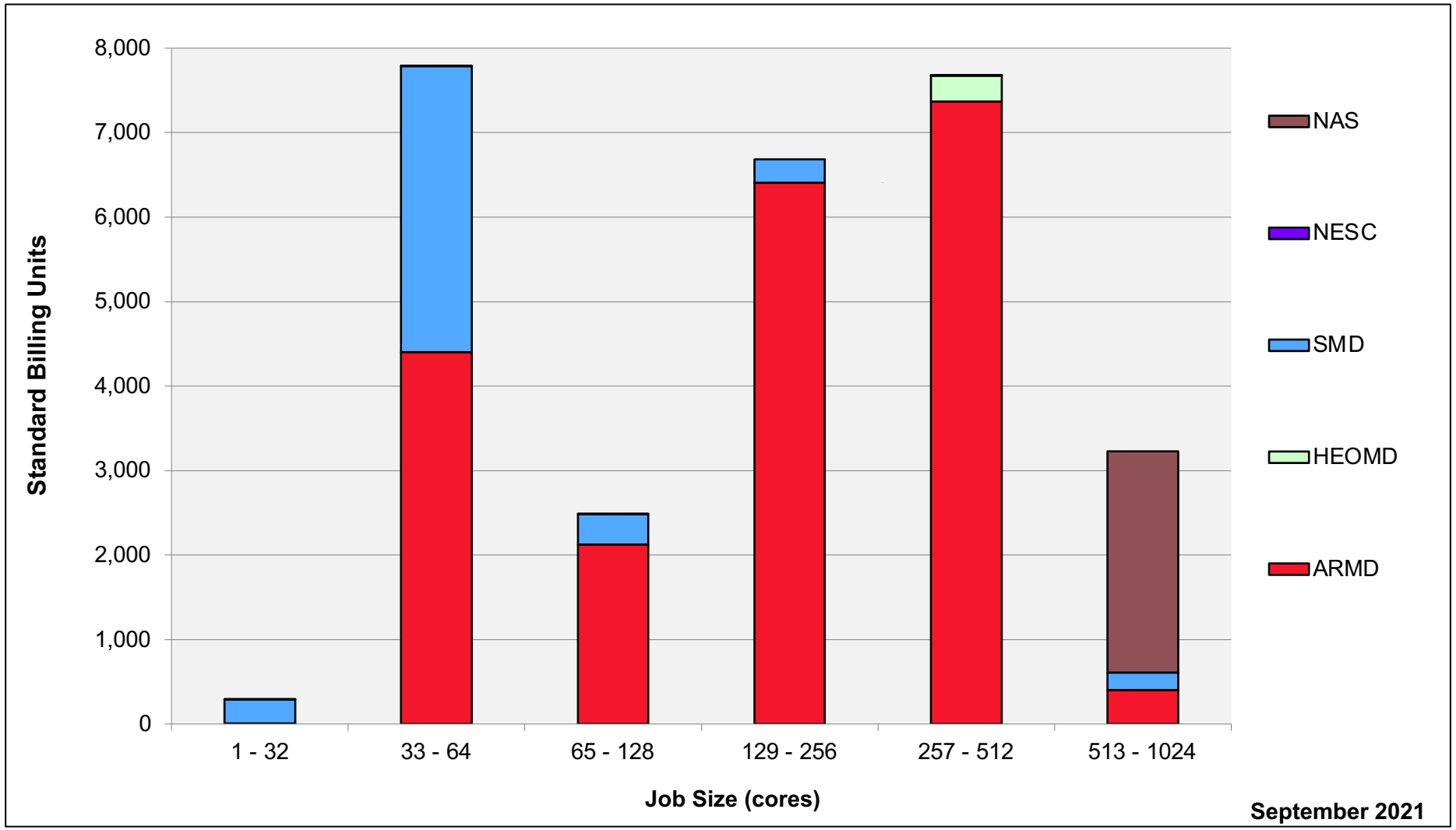
Endeavour: SBUs Reported, Normalized to 30-Day Month



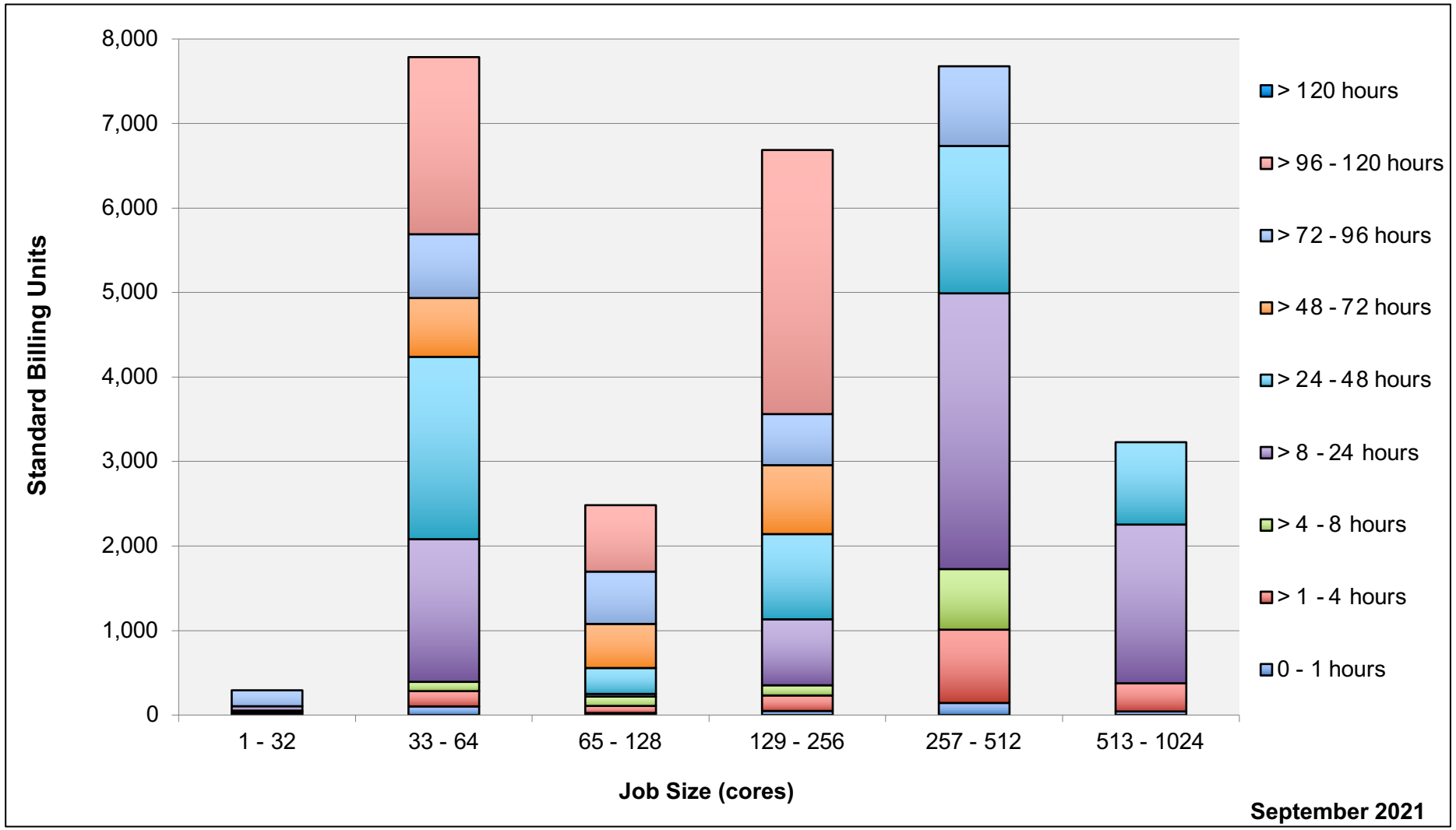
Endeavour: Monthly Utilization by Job Length



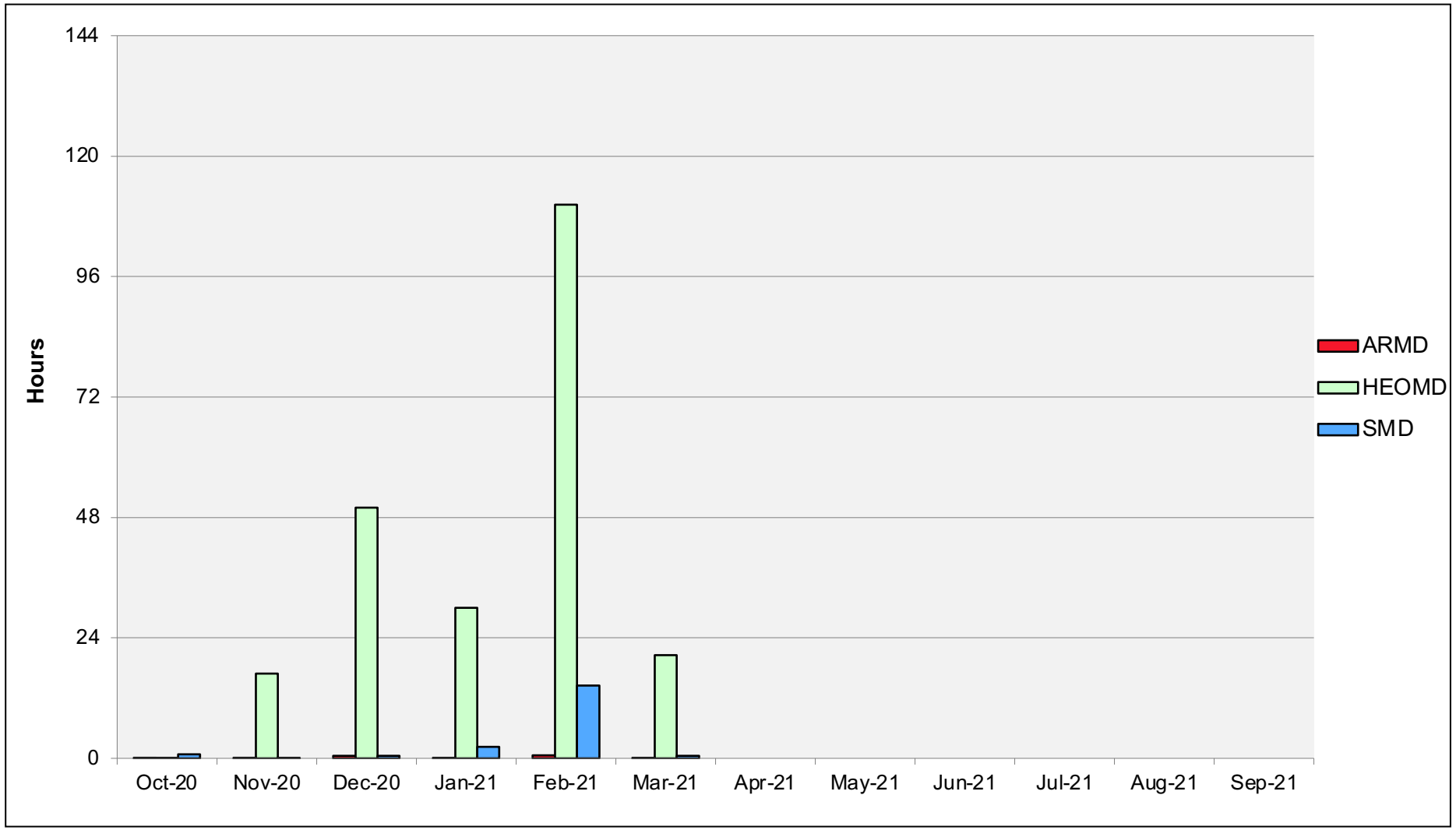
Endeavour: Monthly Utilization by Job Size



Endeavour: Monthly Utilization by Size and Length



Endeavour: Average Time to Clear All Jobs



Endeavour: Average Expansion Factor

