

National Aeronautics and Space Administration

High-End Computing Capability

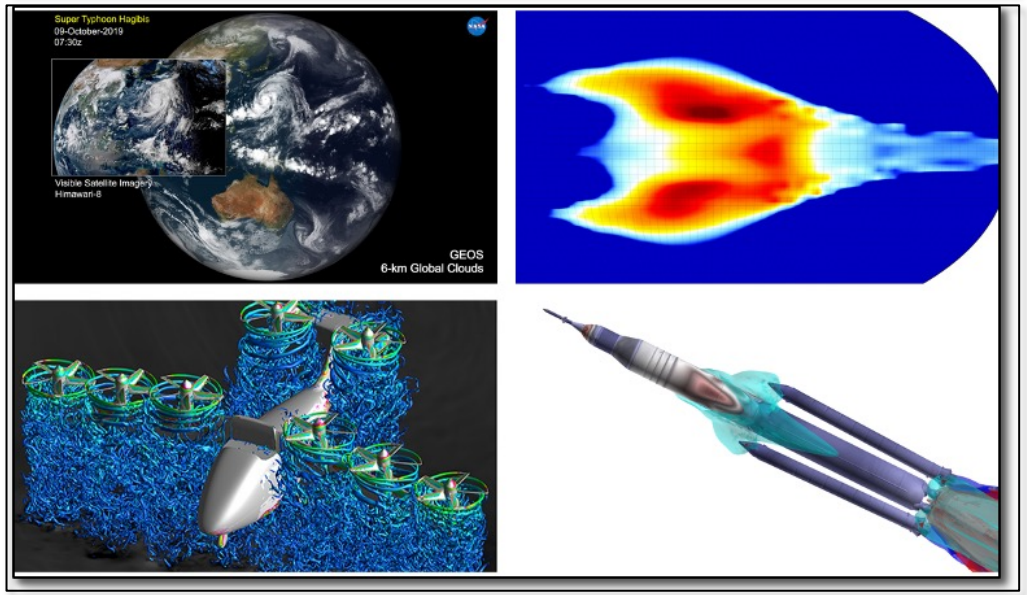
William Thigpen
HECC Component Manager
william.w.thigpen@nasa.gov

November 10, 2023

New Allocation Period for Supercomputer Time Begins for NASA Mission Directorates

- The new operational period (NOP) for all NASA mission directorates began October 1, 2023.
- NAS projects were awarded separate allocations for standard X86 systems (CPU) and accelerated (graphics processing unit (GPU)) resources. Due to the differences between the two architectures, allocations are not interchangeable.
- Mission directorates allocated about 175.5 million Standard Billing Units (SBUs) of standard resources and 200 million SBUs of accelerated resources to 651 projects.
  - The Aeronautics Research Mission Directorate allocated over 10 million CPU SBUs and 27 million GPU SBUs to 134 projects.
  - The Exploration Systems Development, Space Operations, and Space Technology mission directorates, and the NASA Engineering and Safety Center, collectively allocated more than 50.8 million CPU SBUs and 75 thousand GPU SBUs to 77 projects.
  - The Science Mission Directorate allocated more than 84.5 million CPU SBUs and 186 million GPU SBUs.
- The Request Management System (RMS) ensured a smooth process for principal investigators, allocators, and HECC staff.
  - GPU resources were added to the intake form and a separate call for requests was issued as part of the NOP process.

IMPACT: NASA programs and projects periodically review the distribution of supercomputer time to assess demand for resources and assure consistency with mission-specific goals and objectives.



Clockwise from left: Comparison of a satellite image of cyclone Hagibis with an image produced with the experimental GEOS model; Surface air temperature of Proxima Centauri b; Visualization of the flow of NASA's six-passenger tiltwing concept for urban air mobility; Isometric view of the Block 1B Space Launch System vehicle during booster separation.

** 1 SBU represents the work that can be done in 1 hour on a Pleiades Broadwell 28-core node.*

New Apollo Milan Racks Arrive at the NAS Facility

- Four new HPE Apollo 9000 racks with AMD Milan processors were delivered and connected to the NAS facility (building N258) infrastructure on October 30–31.
  - The racks were installed in N258, Room 131. The room was formerly a Sensitive Compartmented Information Facility (SCIF) prior to housing a quantum computer and had the available power and cooling capacity for the new racks.
  - The new racks weigh 4,300 lbs. each and exceed the floor load rating of the N258/230 main computer room raised floor. Room 131 is on the first floor of N258, and the racks rest directly on the room's concrete subfloor.
- Facility upgrades were required to prepare the room for the Milan racks.
  - New electrical cables were installed to power each rack. Each rack has a maximum power draw of 108 kilowatts and is fed through two 100-amp circuit breakers at an input voltage rating of 480 volts.
  - A new overhead cable tray was installed to route the electrical cables from the electrical panel to the racks because there is no raised floor to bring utilities from below as in N258's main computer room.
  - Cooling for the new racks was provided by Room 131's existing cooling pipes with a fine mesh strainer added to protect the plate heat exchanger for the Milan racks.
- The new Milan racks will only temporarily use N258 as their home. They will be moved to the new R&D099 Compute Module 2 in late spring 2024.

IMPACT: The new Milan racks will add 512 nodes (65,536 cores) to HECC resources when fully released to users.

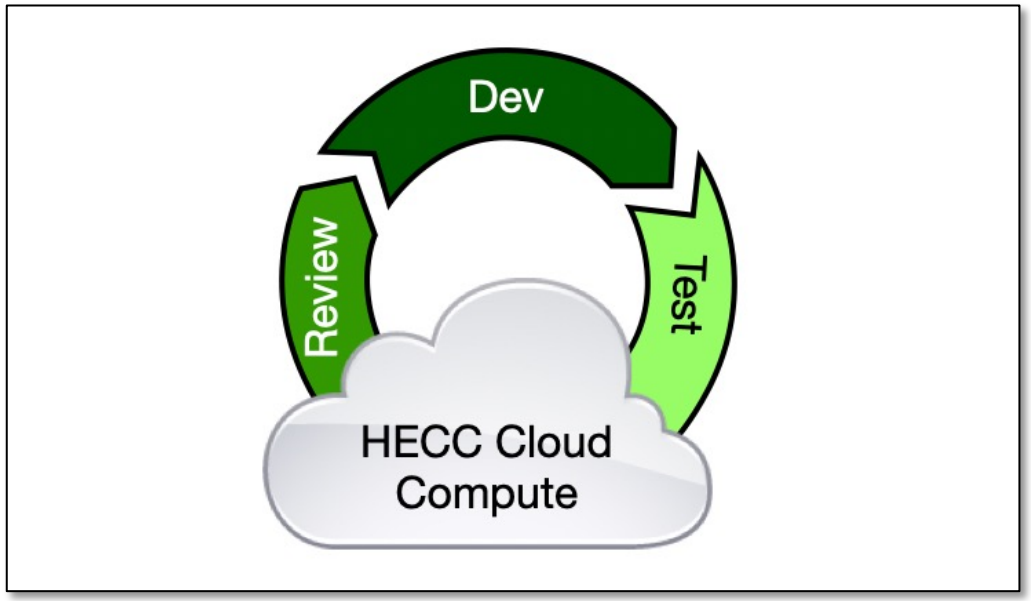


The new Apollo Milan racks are powered up at the NASA Advanced Supercomputing (NAS) facility and ready for initial diagnostic testing. They will be relocated to the Modular Supercomputing Facility at Ames in spring 2024. *Chris Tanner, NASA*

HECC Cloud Environment Improves Software Development/Test Cycle

- The Launch, Ascent, and Vehicle Aerodynamics (LAVA) team leveraged the NAS Amazon Web Services (AWS) cloud offering and were able to rapidly iterate on their software tools and reduce the development/test cycle when making changes and running large-scale cases.
- The team ran 125 jobs during a two-week period, with a typical job size of 64 Intel Skylake nodes. Several jobs used on the order of 100 nodes, which is comparable to on-premise workloads.
- Requesting 64 to 150 Intel Ice Lake nodes (AWS instance type hpc6id) per computational fluid dynamics (CFD) case, the team only had to wait a few minutes to have the nodes ready to use, even when asking for multiple CFD cases. In contrast, the team reports they must routinely wait many days to weeks for single jobs on-prem.
- In addition, the team was able to experiment with modern computing hardware not yet available on HECC systems.
- The team reported that "rapid availability of compute resource is a game changer for productivity and the HPC environment in AWS… is extremely user friendly."

IMPACT: Providing HECC users with readily available, scalable, and user-friendly cloud compute resources on demand creates an opportunity for teams to advance needed software to better meet NASA's mission requirements.

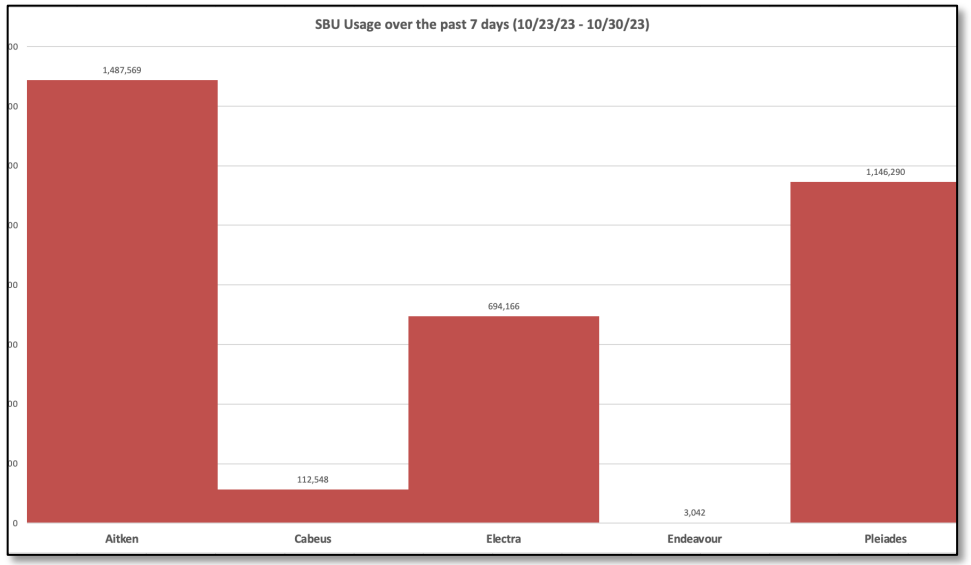


Cloud compute's role in accelerating the development cycle.

Tools Team Implements GPU Accounting System

- The HECC Tools team developed and implemented a new script for parsing PBS log information to account for GPU usage and establish allocation charging. The new script is:
  - Written in a modern programming language for better maintenance.
  - Designed to accommodate changes to architecture to support the dynamic HECC computing environment.
  - Using proven techniques ensure the code is maintainable and modifiable as personnel change over the years.
- The script supports the use of single GPUs, instead of the full node.
  - The GPUs nodes are configured to allow for sharing of the nodes for running jobs. The new script supports the various types of configuration so that users are only charged per GPU utilized.
  - This allows users to efficiently use their allocation, using only what they need while allowing more users to access the GPU environment.
- A new separate GPU allocation was created to manage and track GPU-specific requests and usage.
  - Having separate allocations for GPU vs. CPU simplifies usage tracking for both HECC management and GPU users.
- The command line tool was updated to provide support for “Account Query” and “Account Year to Date” queries.

IMPACT: The new system allows users to understand how much of their allocations they are using on the GPUs on the PBS server pbspl4 and enables HECC management to understand utilization trends for the GPUs.

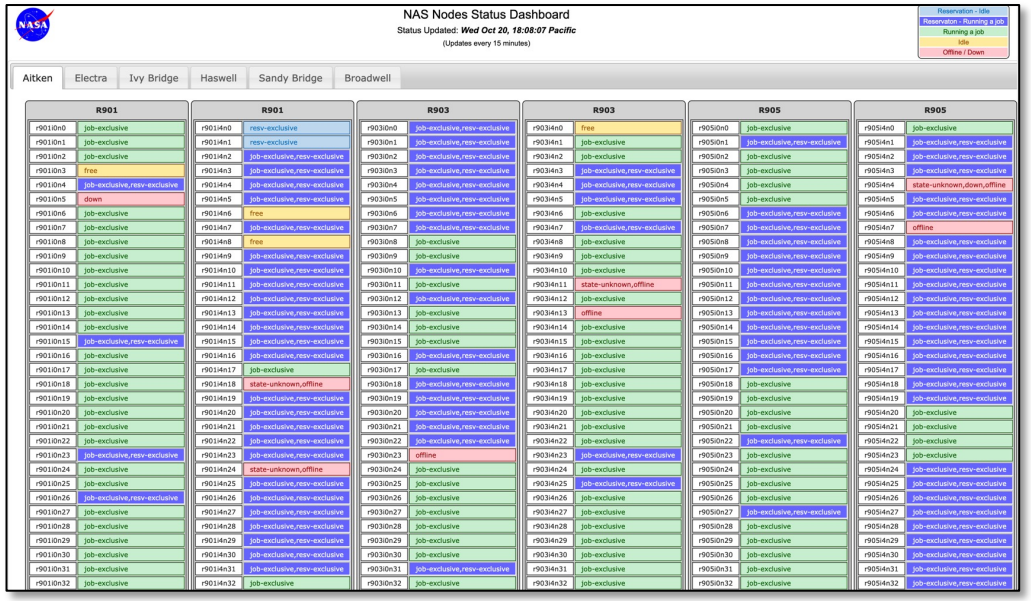


SBU usage reported by the new script from 10/23/23 to 10/30/23 displays Cabeus GPU utilization with other systems. The graph shows utilization in SBUs for Aitken (1,487,569), Cabeus (112,548), Electra (694,166), Endeavour (3,042) and Pleiades (1,146,290).

New Nodes Status Dashboard Completed

- The HECC Tools team developed the NAS Nodes Status Dashboard, a web tool that enables Control Room analysts to rapidly assess, at a glance, the status of compute nodes at the NAS facility.
  - Nodes are visually displayed in their physical rack positions.
  - Updates occur automatically every 15 minutes.
  - The design is based on a spreadsheet previously used by NAS system analysts.
- The dashboard's features include:
  - Tabs to navigate to the major compute clusters and/or node architectures.
  - Color-coding of node statuses for reserved, running, idle, and offline states.
  - Per-rack displays of node counts in various states.
  - The ability to drill into counts of offline nodes for more detailed analysis.
- The dashboard uses Perl and shell scripts on the back end to process node status data, and the jQuery JavaScript library for the front-end client application.
- The Tools team is planning future enhancements, including:
  - The ability to highlight changed states from one day and two days prior.
  - The option to view by node architecture for all the compute clusters.

IMPACT: The new node status dashboard displays NAS compute nodes arranged in their physical rack locations, facilitating the rapid discovery of spatial relationships of node faults and behaviors.



Screenshot of a portion of the NAS Node Status Dashboard. The various compute clusters are accessed via tabs. *Glenn Deardorff, NASA/Ames*

Powering Synthetic Data Generation with HPC and Dask*

- To better understand the observational data of phytoplankton, the Biospheric Science team at NASA Ames developed the Spectral Water Inversion Processor and Emulator (SWIPE) tool, which uses synthetic data to help model and analyze of the optical properties of water containing algae.
- Because generating synthetic data is time consuming—SWIPE takes over two hours on a laptop to complete an analysis of just one species of phytoplankton—the Biospheric Science team reached out to the NAS Data Science team to help speed up the process.
  - The Data Science team embedded Dask—a flexible open-source Python library for parallel computing—into the SWIPE tool to allow the distribution of the EAP code across multiple processors and nodes on the Pleiades supercomputer.
  - Using the Dask framework allowed the scientists to use modules such as "dask.delayed" to run SWIPE's EAP code in parallel, increasing the number of processors allocated to the job. This reduced the dataset generation time to about 18 minutes using Pleiades, compared to two hours on a laptop.
- Leveraging the power of Pleiades and code parallelization, the two teams were able to increase the rate of dataset generation sixfold, which would not have been possible without access to NASA high-performance computing resources and knowledgeable support staff.

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

IMPACT: Using HECC resources and data science expertise significantly reduced the Ames Biospheric Science team's time-to-solution for computing spectral data of phytoplankton species.

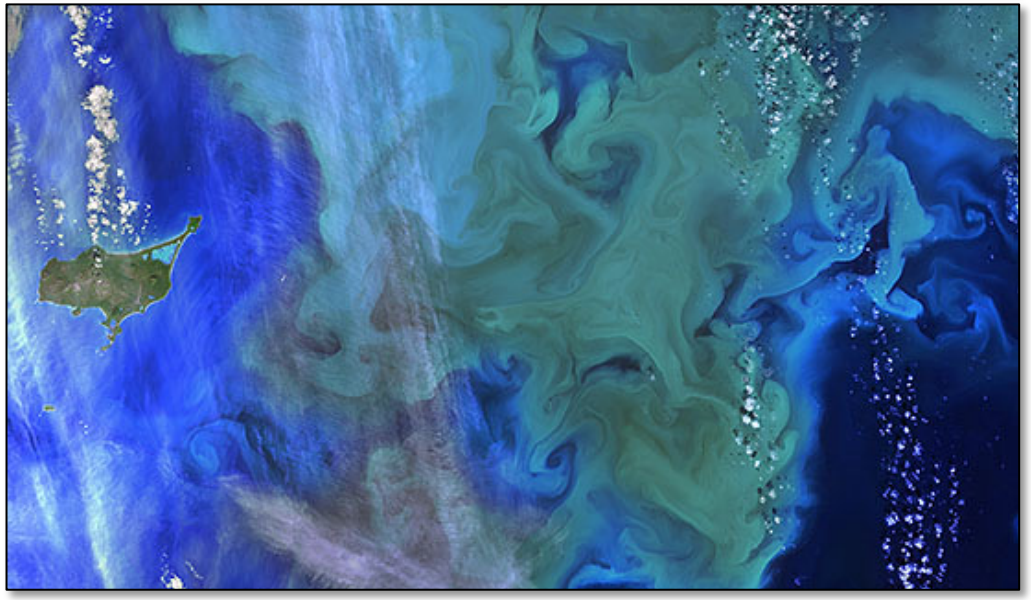


Image composite from Landsat 8 data captured September 22, 2014 shows a phytoplankton bloom (green and blue swirls) near the Pribilof Islands off the coast of Alaska in the Bering Sea. The turquoise waters are likely colored by a type of phytoplankton called coccolithophores. *Norman Kuring, NASA/Goddard*

Papers

- "**Not all Spacetime Coordinates for General-Relativistic Ray Tracing are Created Equal**," G. Bozzola, C.-K. Chan, V. Paschalidis, *Physical Review D*, vol. 108, issue 8, published online October 3, 2023. *
  https://journals.aps.org/prd/abstract/10.1103/PhysRevD.108.084004
- "**Comptonization by Reconnection Plasmoids in Black Hole Coronae II: Dependence on the Guide Field in Pair Plasma**," S. Gupta, N. Sridhar, L. Sironi, arXiv:2310.04233 [astro-ph.HE], October 6, 2023. *
  https://arxiv.org/abs/2310.04233
- "**Not-so-Fast Kepler-1513: A Perturbing Planetary Interloper in the Exomoon Corridor**," D. Yahalomi, et al., *Monthly Notices of the Royal Astronomical Society*, vol. 527, issue 1, published online October 9, 2023. *
  https://academic.oup.com/mnras/advance-article/doi/10.1093/mnras/stad3070/7303293
- "**Simulated Atmospheric Response to Large-Scale Dust Forcing and Implications for Martian Dust Storm Growth**," H. Wang, A. Toigo, M. Richardson, *Journal of Geophysical Research: Planets*, vol. 128, issue 10, published online October 11, 2023. *
  https://agupubs.onlinelibrary.wiley.com/doi/full/10.1029/2023JE007956
- "**On the Origin of the Ancient, Large-Scale Cold Front in the Perseus Cluster of Galaxies**," E. Bellomi, et al., arXiv:2310.09422 [astro-ph.HE], October 13, 2023. *
  https://arxiv.org/abs/2310.09422
- "**JWST-TST DREAMS: Quartz Clouds in the Atmosphere of WASP-17b**," D. Grant, et al., *The Astrophysical Journal Letters*, vol. 956, no. 2, published online October 16, 2023. *
  https://iopscience.iop.org/article/10.3847/2041-8213/acfc3b/meta

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

Papers (cont.)

- "**Asteroid 2023 NT1: A Cautionary Tale**," B. Bailey, et al., arXiv:2310.13112 [astro-ph.EP], October 19, 2023. * https://arxiv.org/abs/2310.13112
- "**Internally Heated and Fully Compressible Convection: Flow Morphology and Scaling Laws**," W. Powers, E. Anders, B. Brown, arXiv:2310.15380 [physics.fly-dyn], October 23, 2023. * https://arxiv.org/abs/2310.15380
- "**New Mass and Radius Constraints on the LHS 1140 Planets—LHS 1140 b is Either a Temperate Mini-Neptune or a Water World**," C. Cadieux, et al., arXiv:2310.15490 [astro-ph.EP], October 24, 2023. * https://arxiv.org/abs/2310.15490
- "**The GAPS Programme at TNG XLIX. TOI-5398, the Youngest Compact Multi-Planet System Composed of an Inner Sub-Neptune and an Outer Warm Saturn**," G. Mantovan, et al., arXiv:2310.16888 [astro-ph.EP], October 25, 2023. * https://arxiv.org/abs/2310.16888
- "**A Lithium Depletion Age for the Carina Association**," M. Wood, et al., arXiv:2310.16883 [astro-ph.SR], October 25, 2023. * https://arxiv.org/abs/2310.16883
- "**Kepler Bonus: Light Curves of Kepler Background Sources**," J. Martinez-Palomera, C. Hedges, J. Dotson, arXiv:2310.17733 [astro-ph.EP], October 26, 2023. * https://arxiv.org/abs/2310.17733

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Papers (cont.)

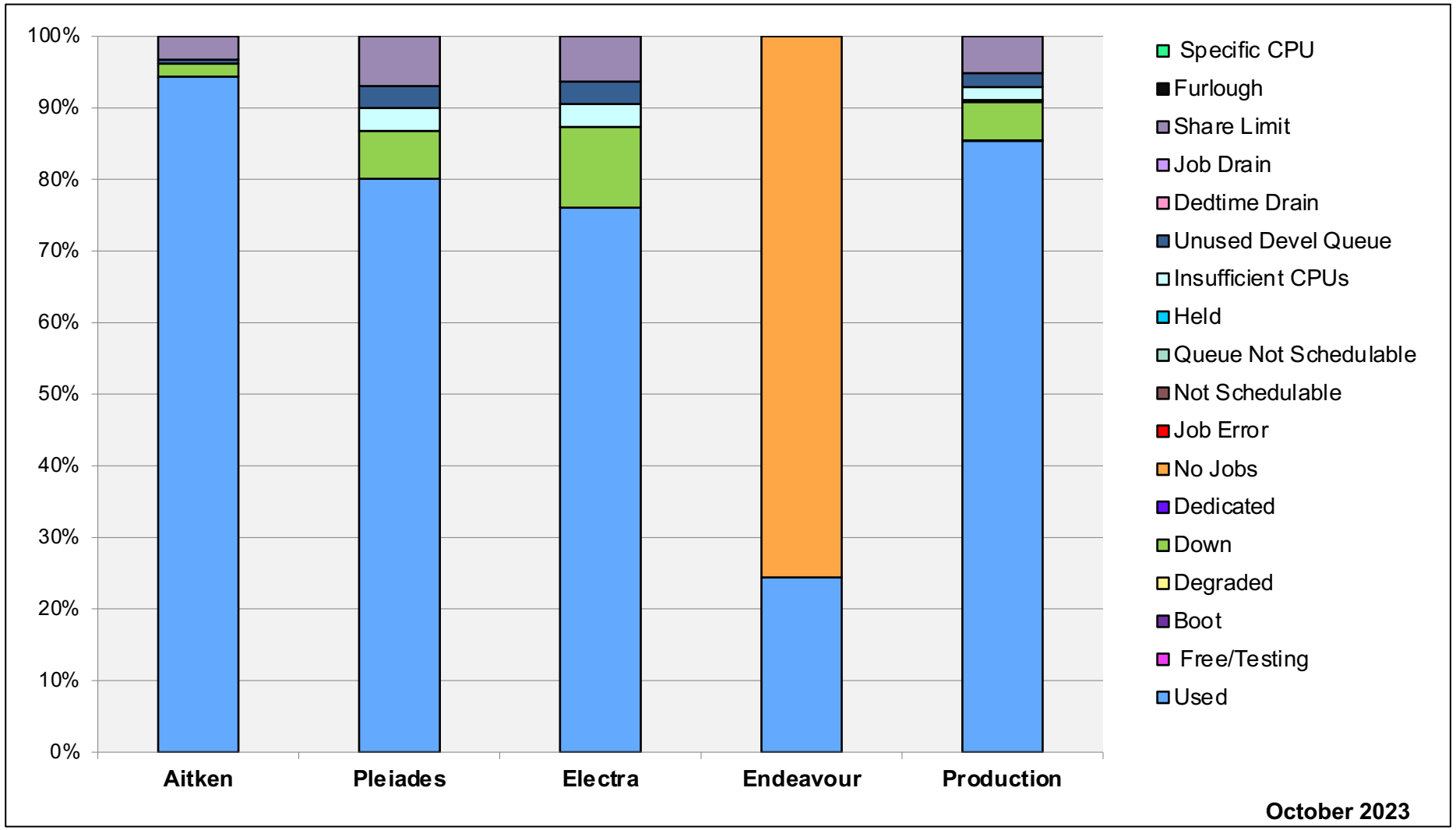
- "**On the Impact of a Dry Intrusion Driving Cloud-Regime Transitions in a Midlatitude Cold-Air Outbreak**," F. Tornow, et al., *Journal of the Atmospheric Sciences*, published online October 27, 2023. *
  https://journals.ametsoc.org/view/journals/atsc/aop/JAS-D-23-0040.1/JAS-D-23-0040.1.xml
- "**Subglacial Discharge Accelerates Future Retreat of Denman and Scott Glaciers, East Antarctica**," T. Pelle, et al., *Science Advances*, vol. 9, issue 43, October 27, 2023. *
  https://www.science.org/doi/full/10.1126/sciadv.adi9014
- "**A Radio Bubble Shredded by Gas Sloshing?**" A. Botteon, et al., *Monthly Notices of the Royal Astronomical Society*, published online October 28, 2023. *
  https://academic.oup.com/mnras/advance-article/doi/10.1093/mnras/stad3305/7332924

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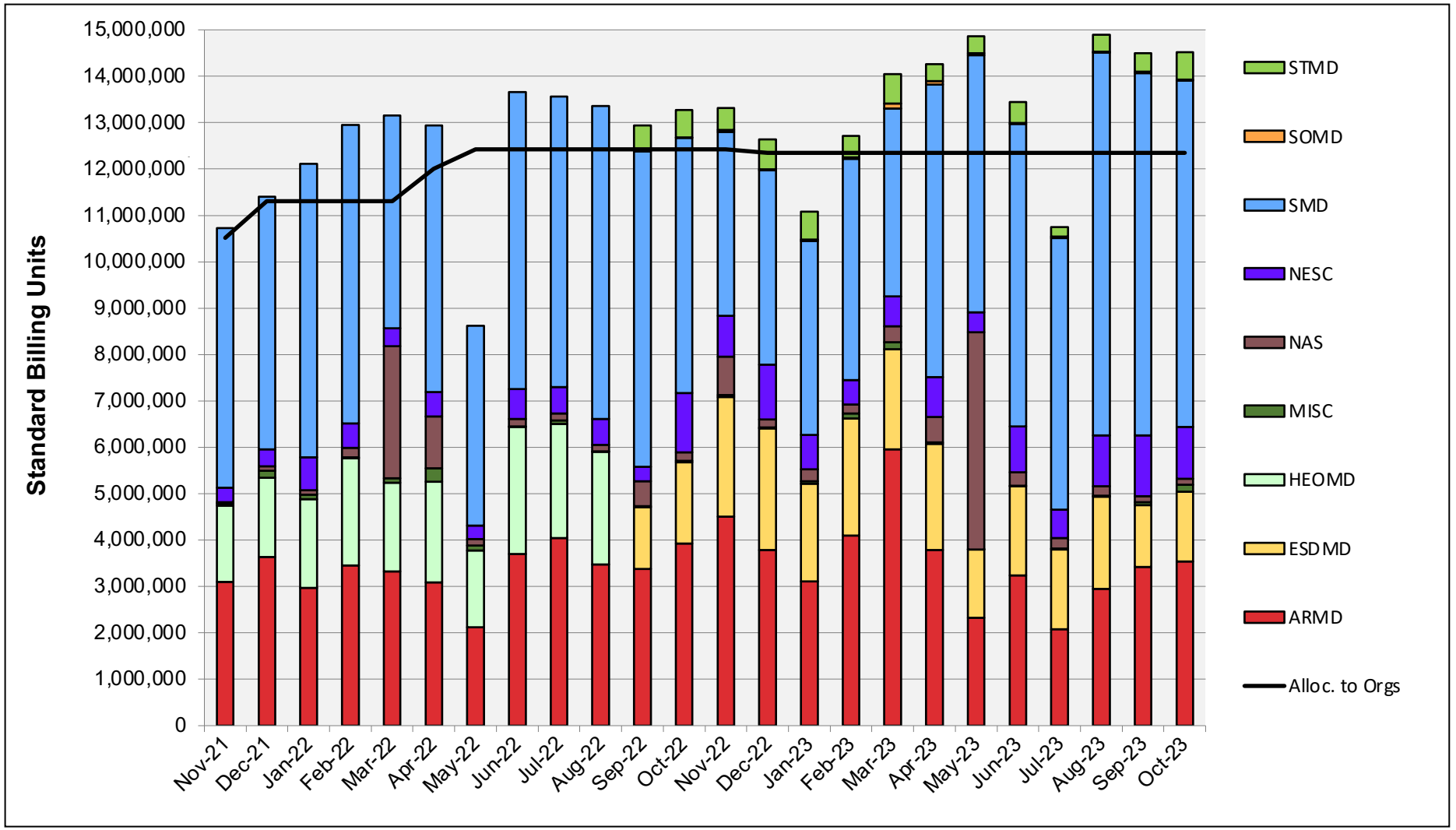
News and Events

- **How NASA is Driving Efficiency with Modular Data Centres**, *Scientific Computing World*, November 3 , 2023—HECC Project Manager Bill Thigpen shares how NASA is driving efficiency with modular data centers, as part of the Breakthrough collection of interviews with Scientific Computing World.
  https://www.scientific-computing.com/article/breakthroughs-2023-how-nasa-driving-efficiency-modular-data-centres
  (*requires registration to read*)
- **Our Moon's Earliest History is Still a Puzzle**, *Forbes*, October 9, 2023—A new paper by researchers from the Southwest Research Institute details a dynamical model to simulate impacts and impactor sources for strikes to the lunar surface early in the Moon's development. To get enough statistics for their model runs, they used the Pleiades supercomputer to get detailed calculations never done before in a coherent, single simulation.
  https://www.forbes.com/sites/brucedorminey/2023/10/09/our-moons-earliest-impact-history-is-still-a-puzzle

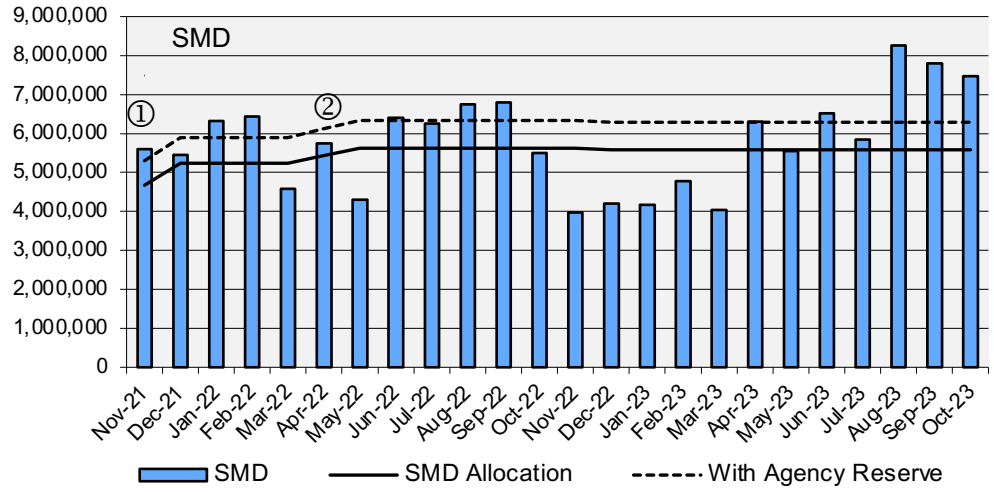
HECC Utilization

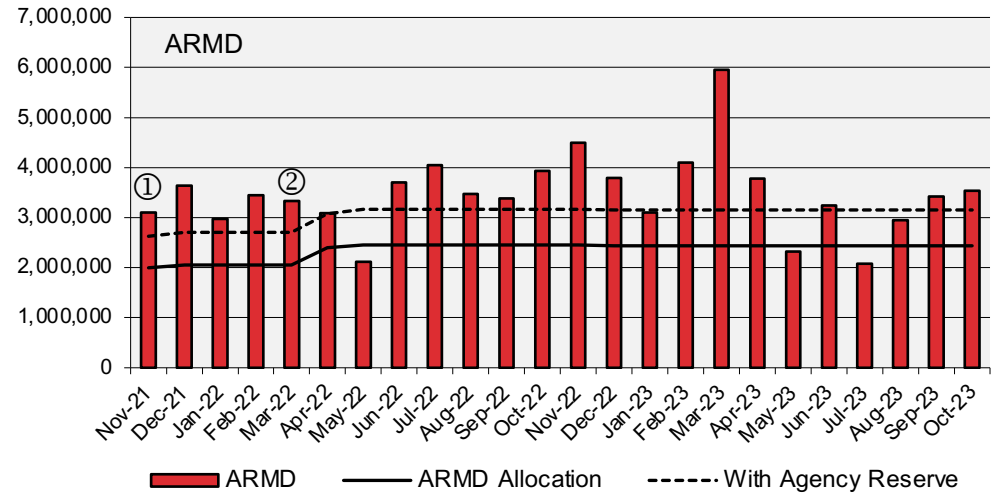


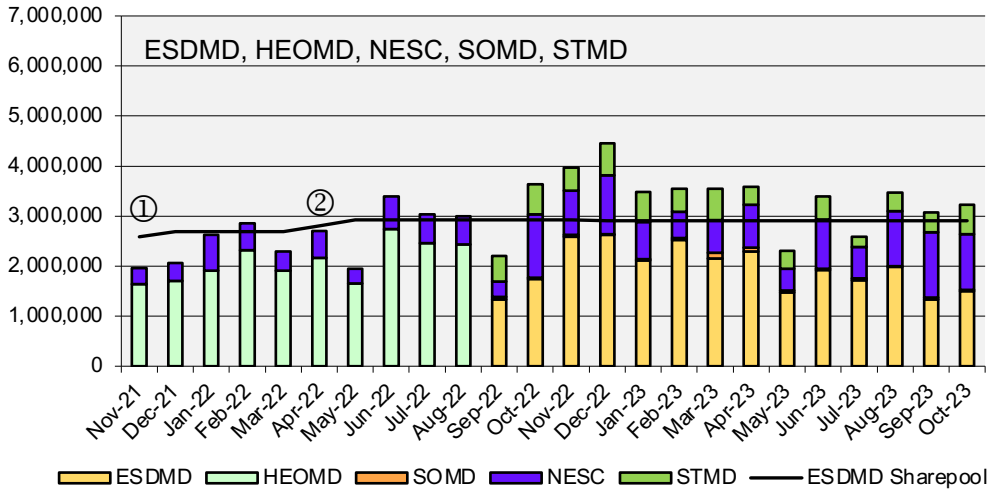
HECC Utilization Normalized to 30-Day Month



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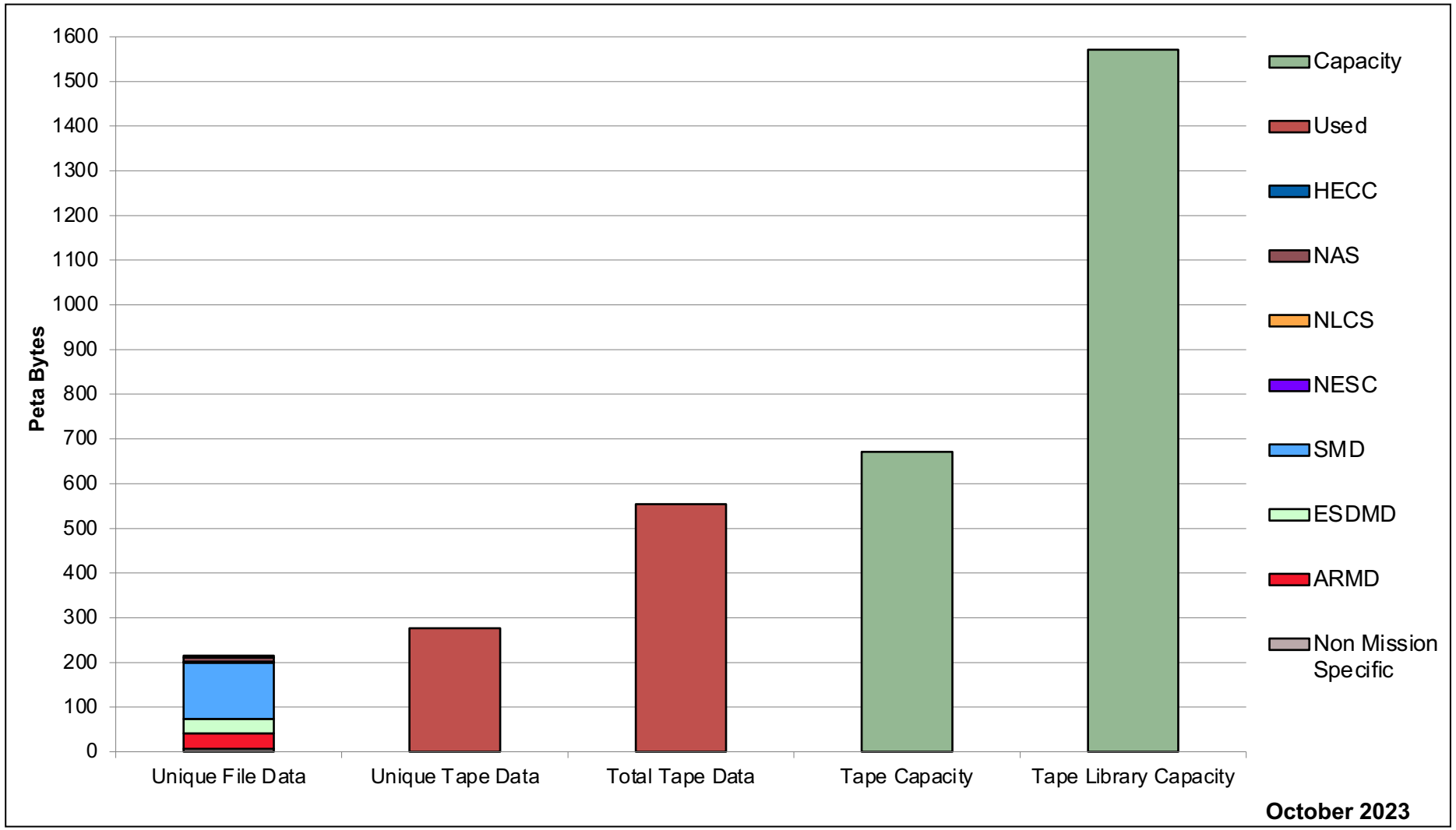




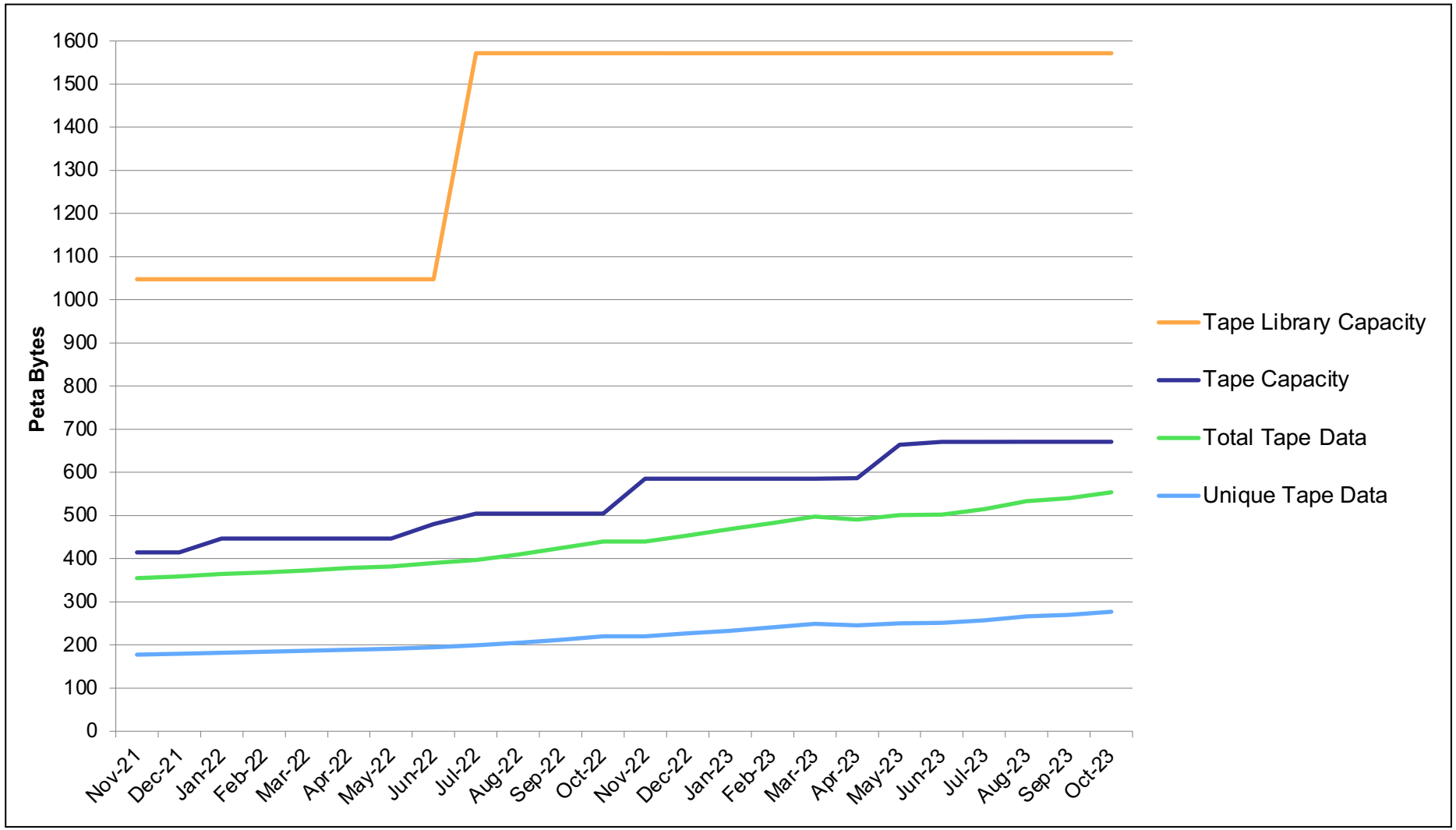
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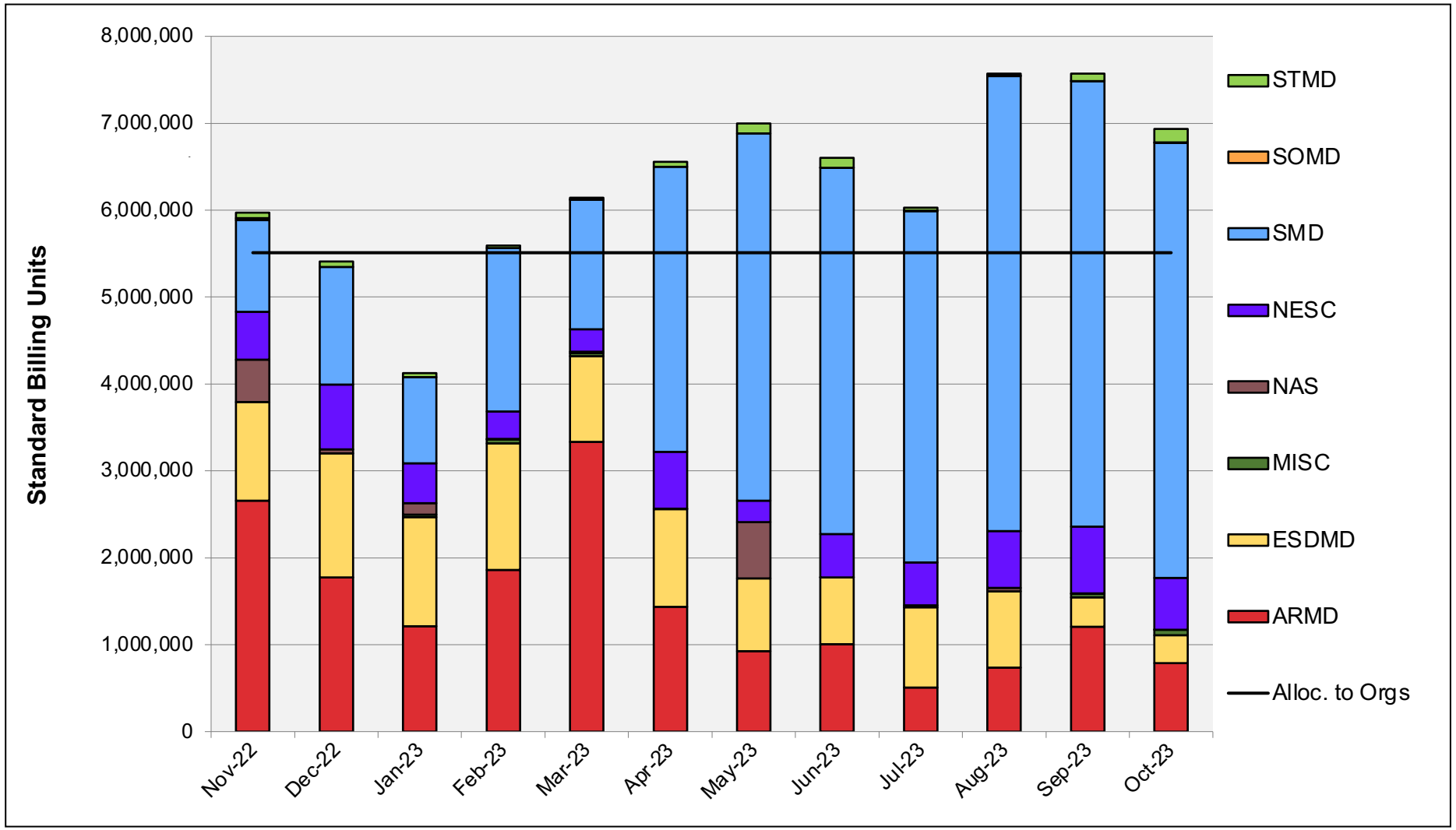
Tape Archive Status



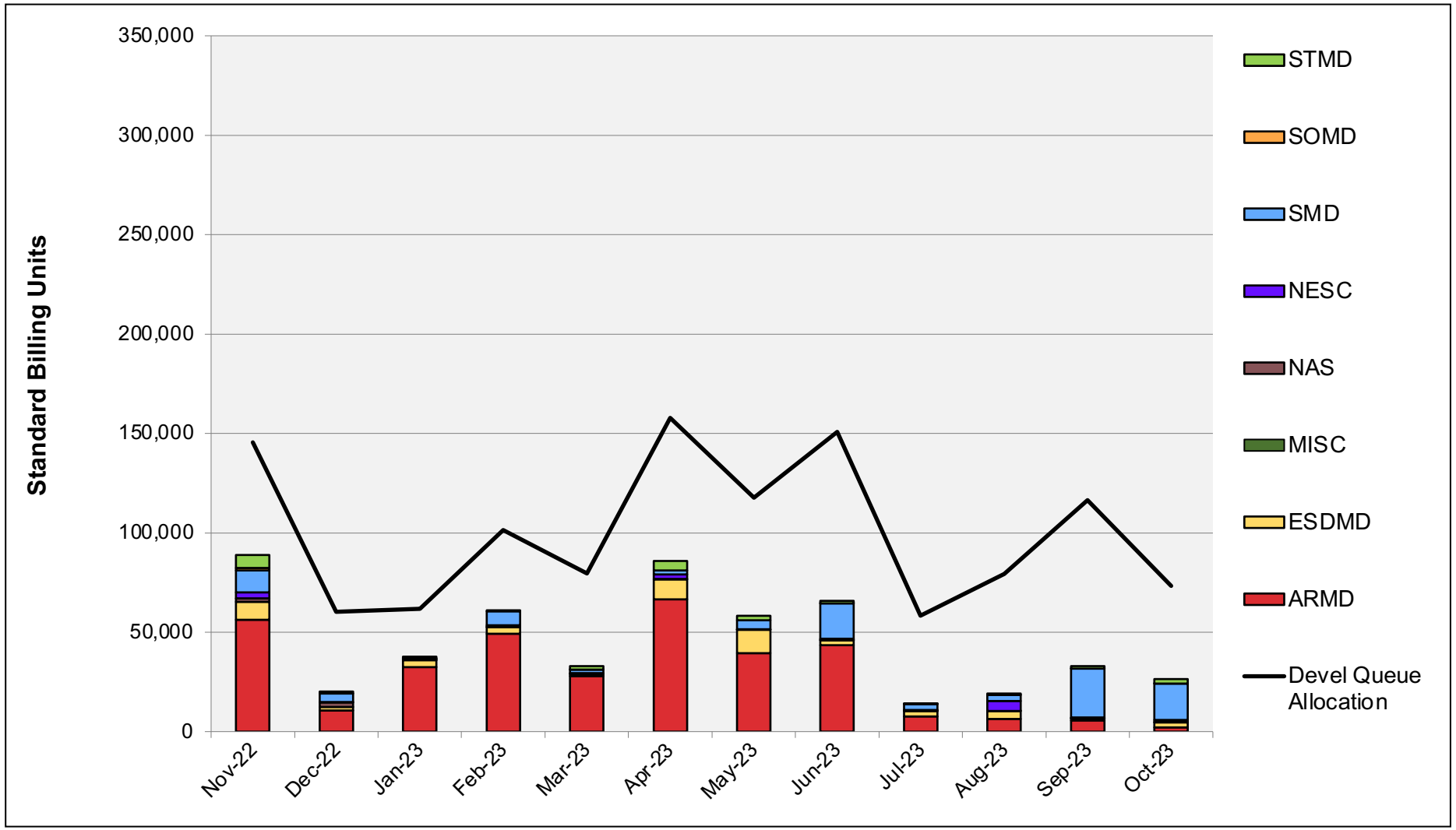
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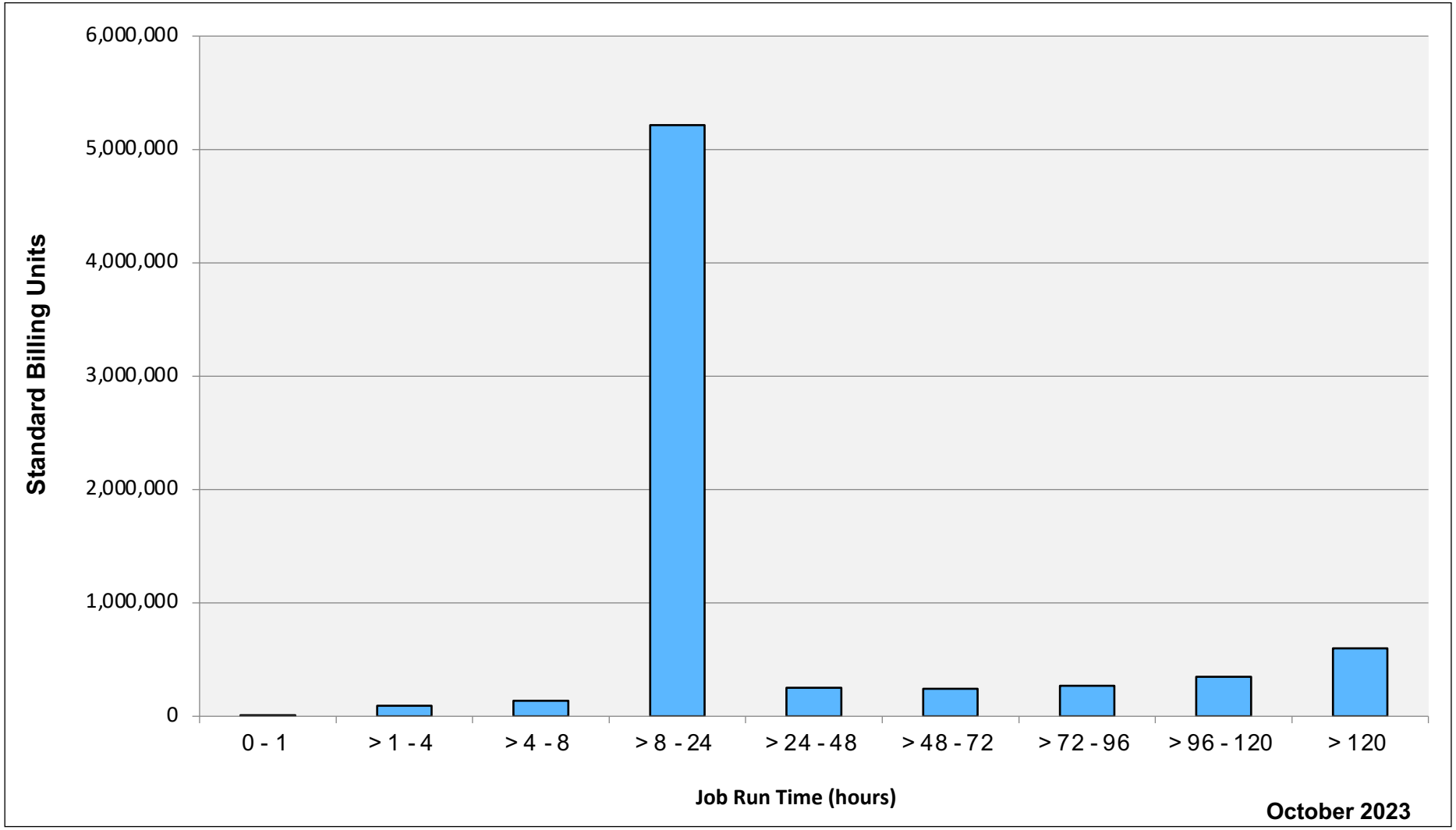
Aitken: SBUs Reported, Normalized to 30-Day Month



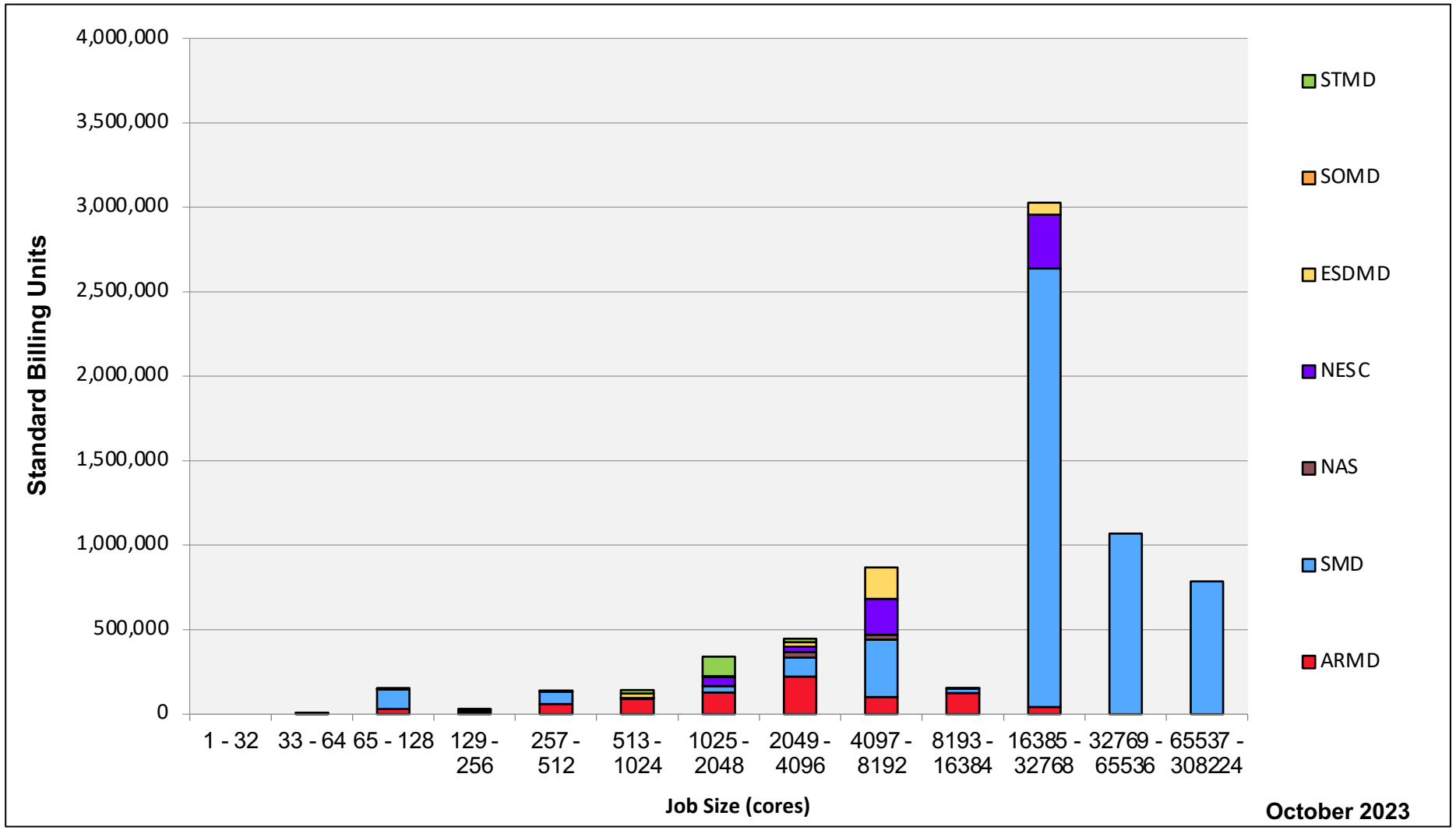
Aitken: Devel Queue Utilization



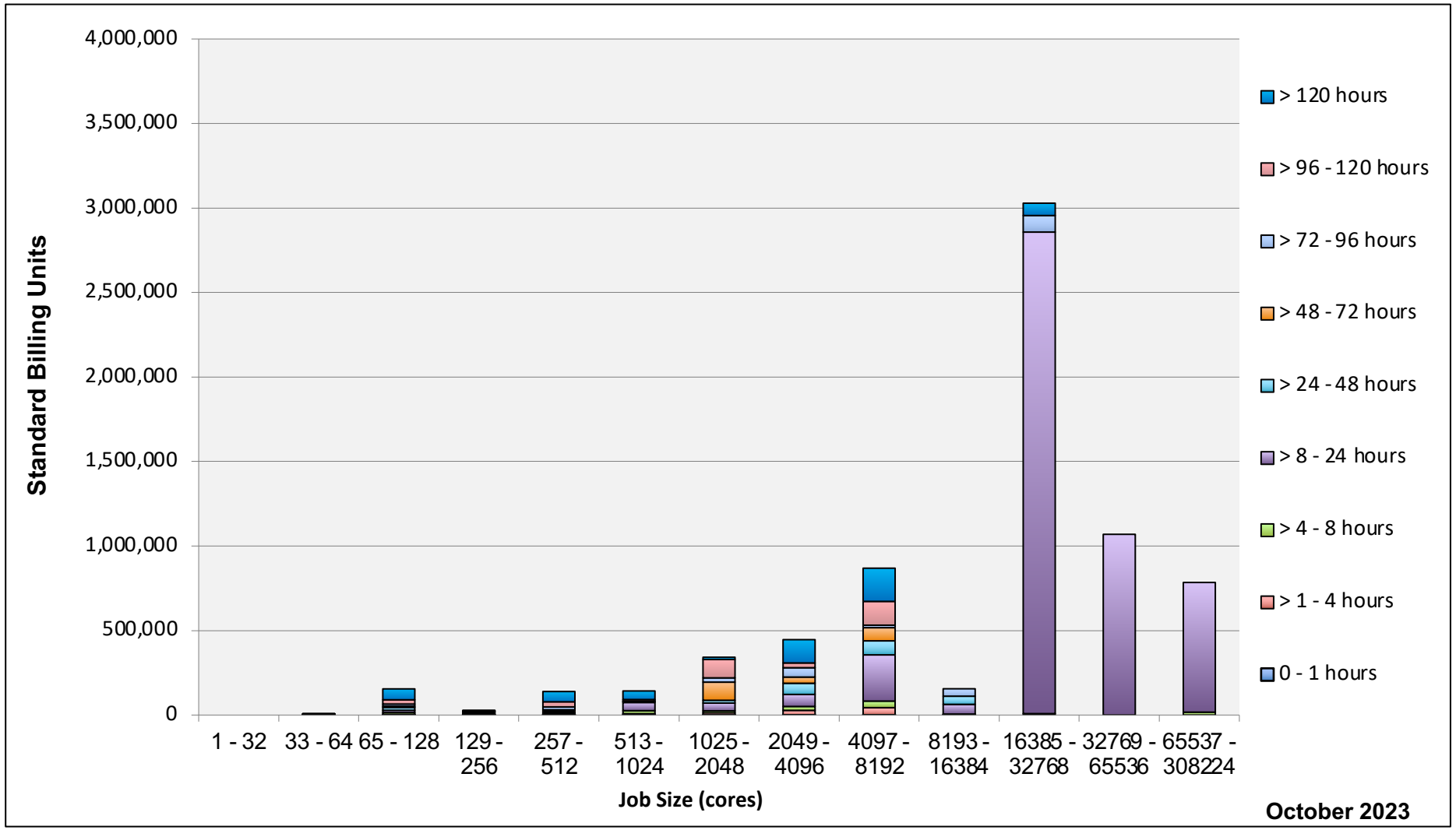
Aitken: Monthly Utilization by Job Length



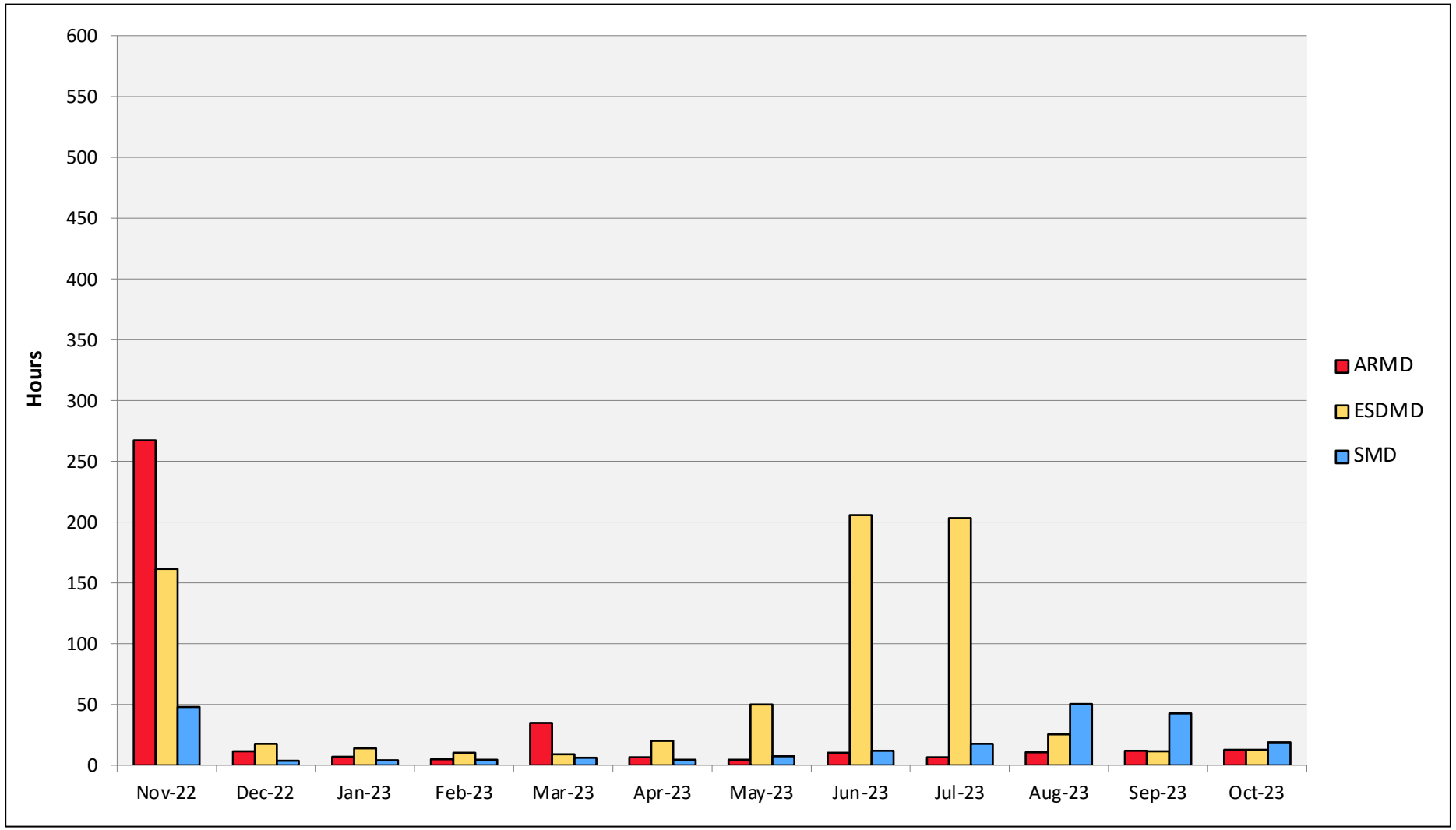
Aitken: Monthly Utilization by Job Size



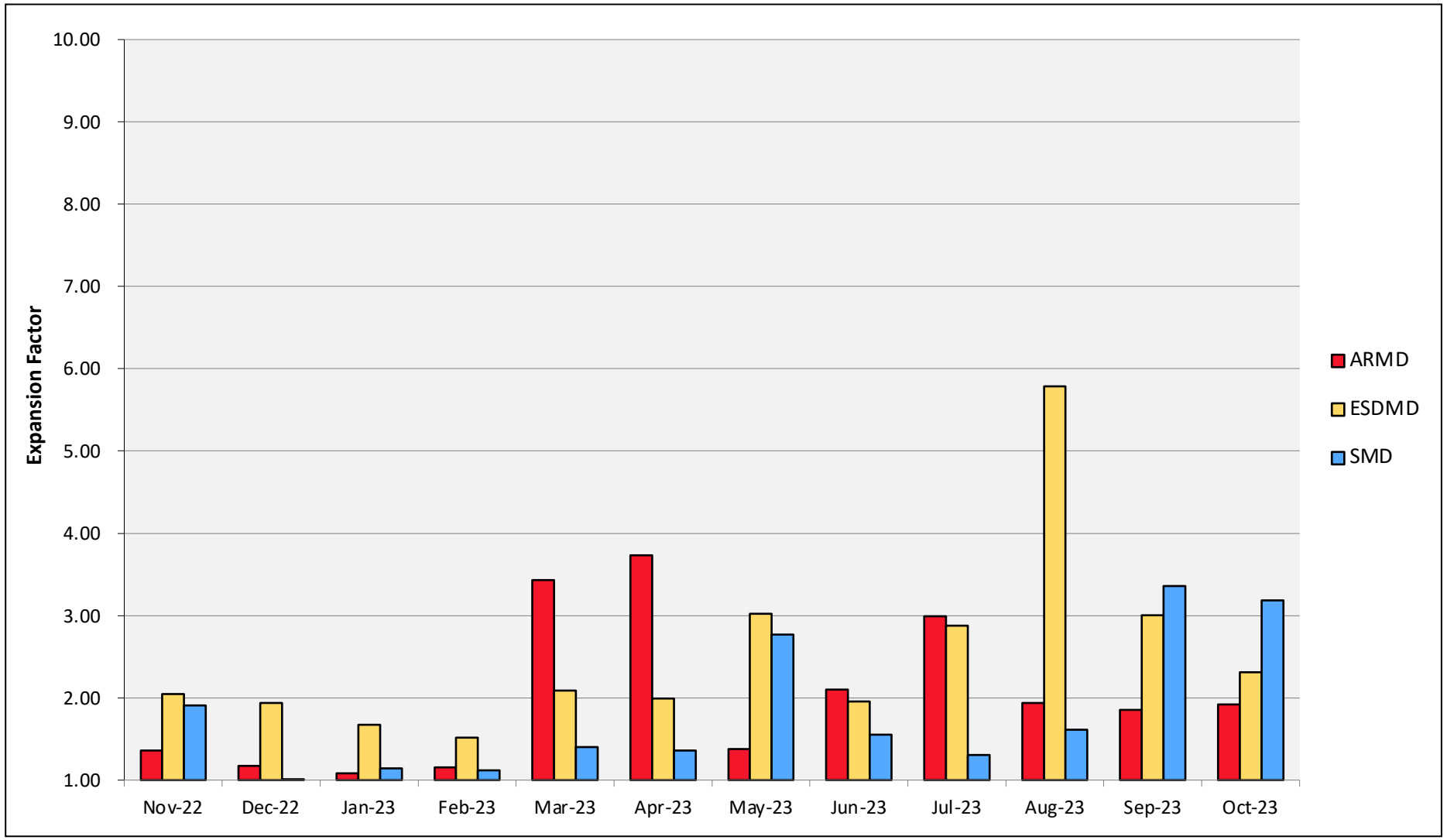
Aitken: Monthly Utilization by Size and Length



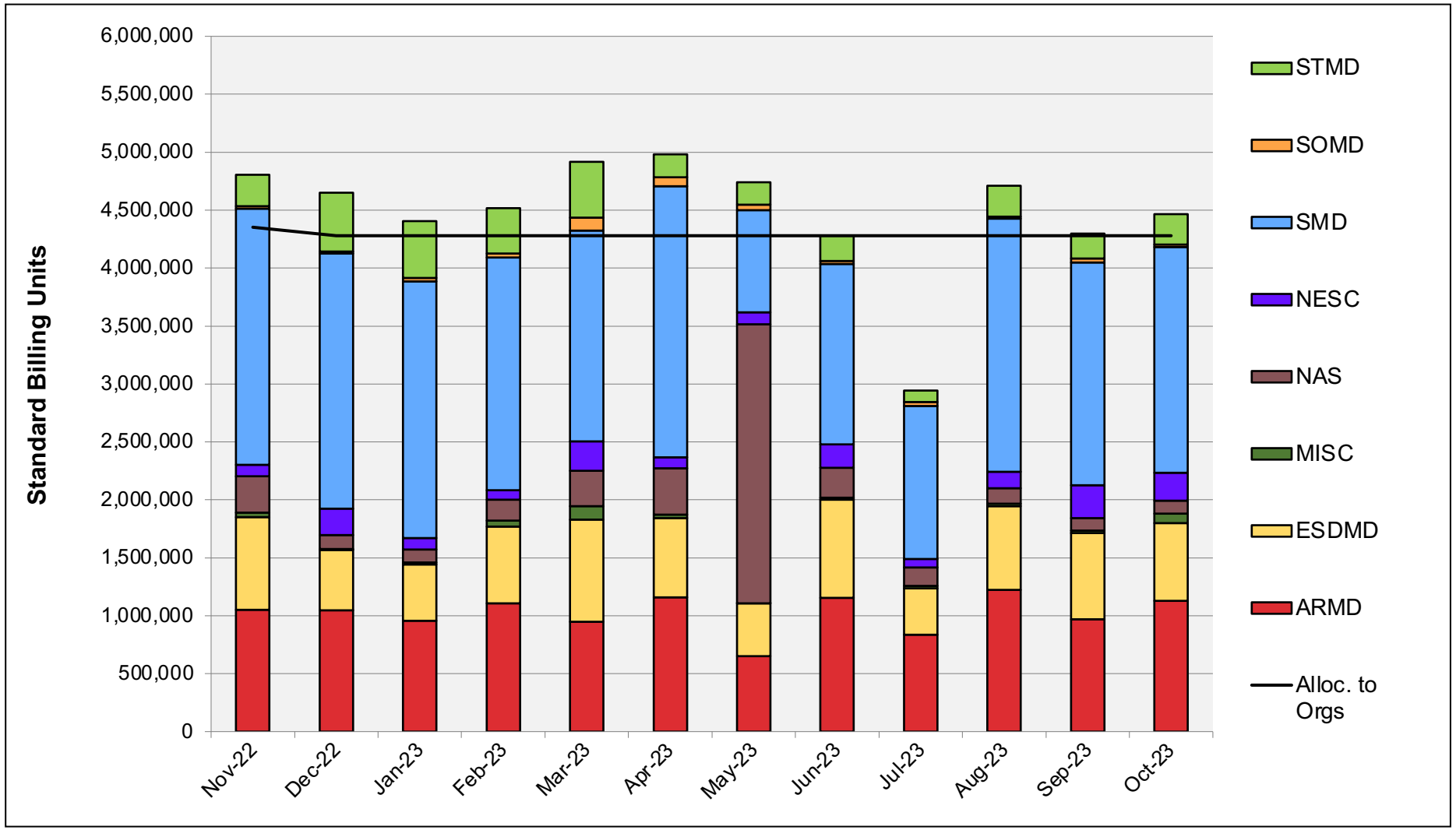
Aitken: Average Time to Clear All Jobs



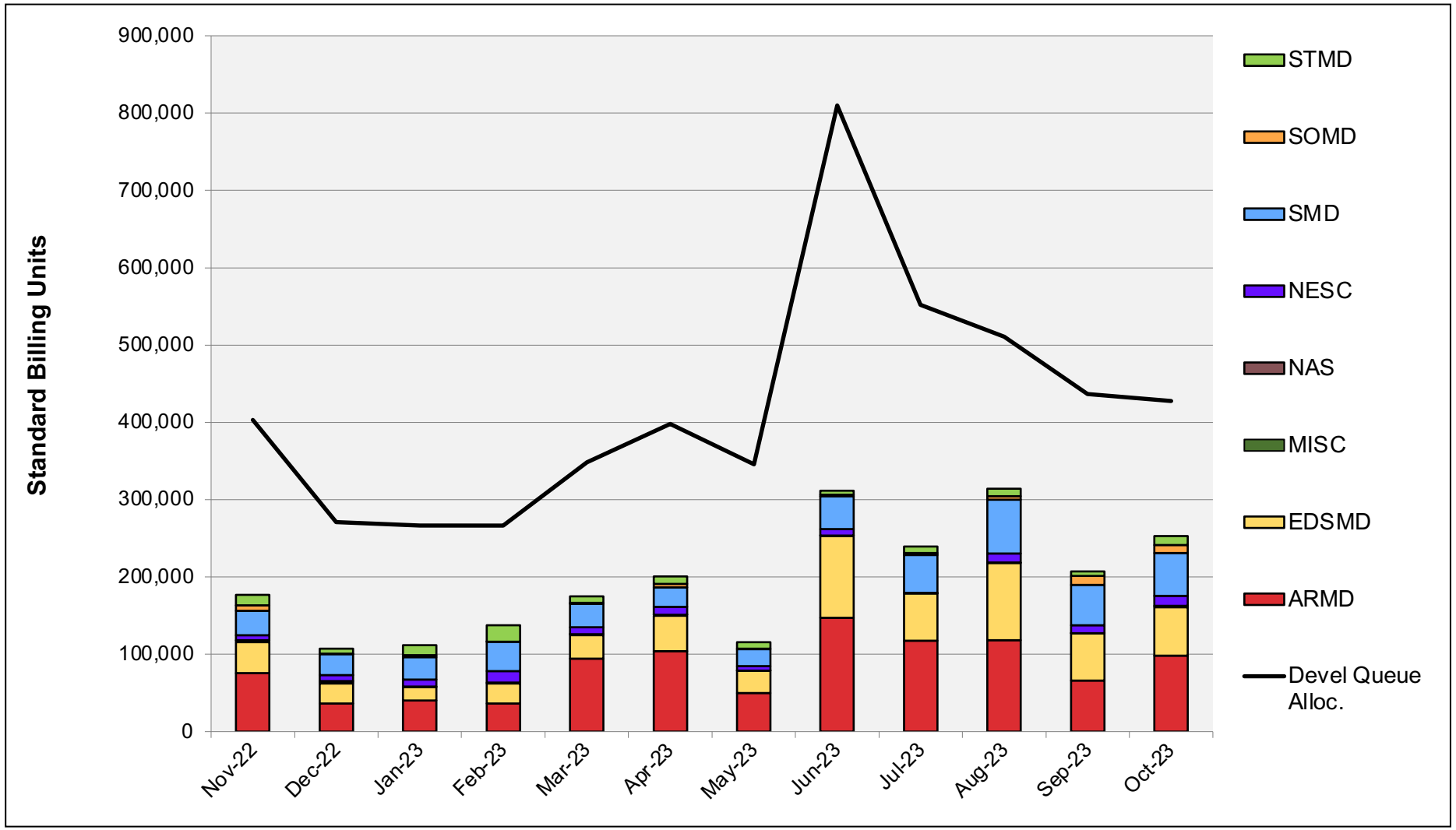
Aitken: Average Expansion Factor



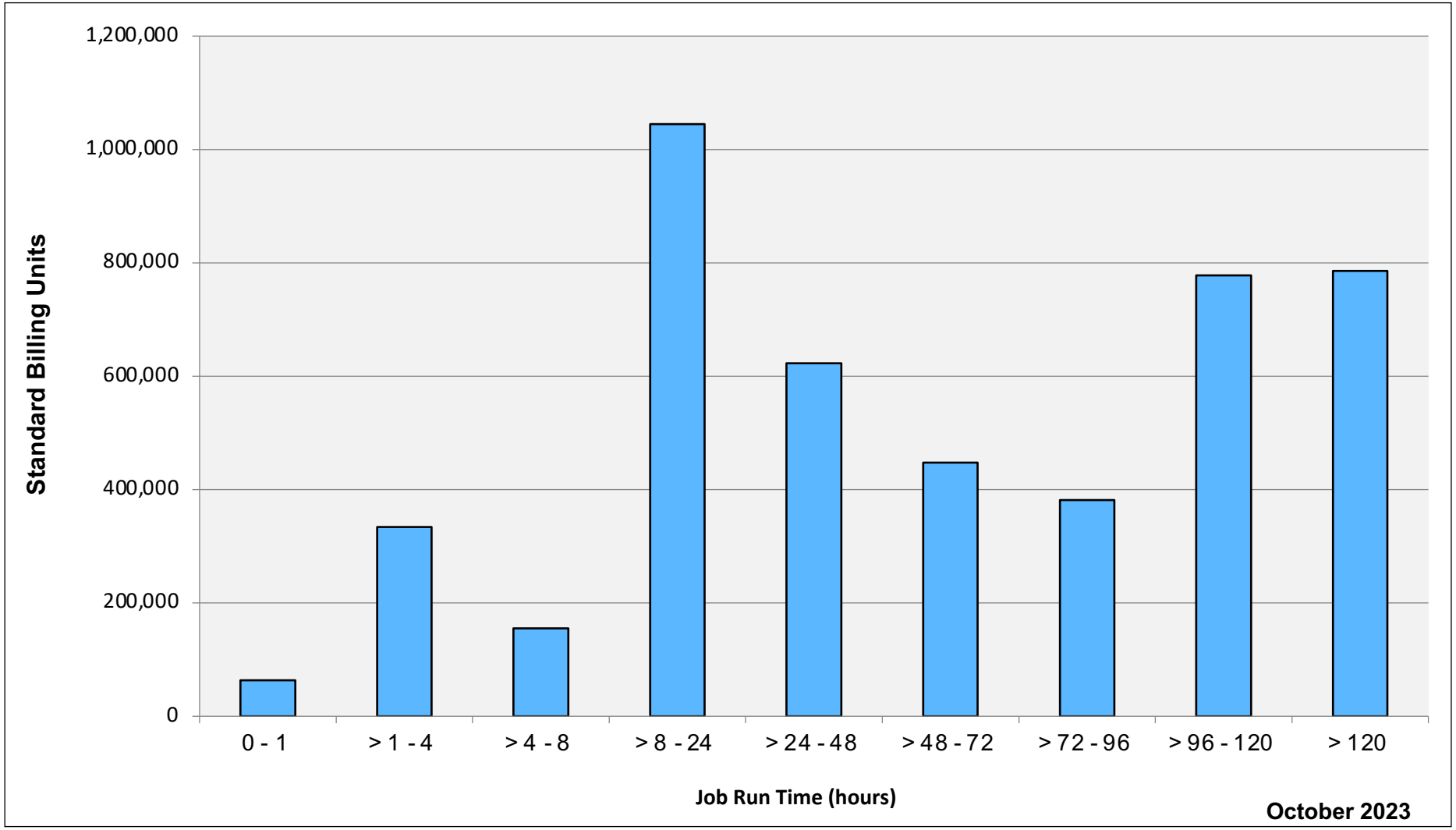
Pleiades: SBUs Reported, Normalized to 30-Day Month



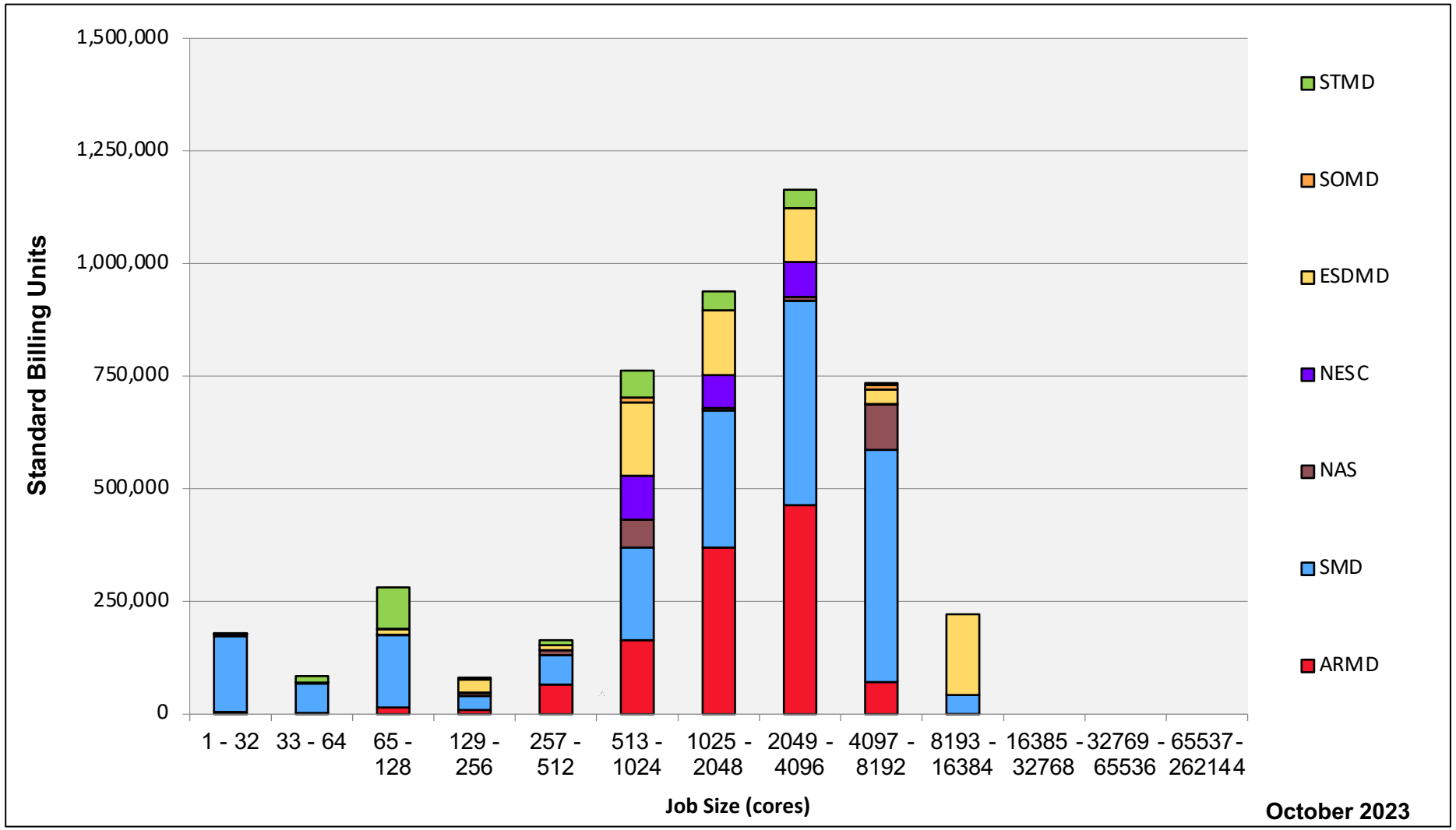
Pleiades: Devel Queue Utilization



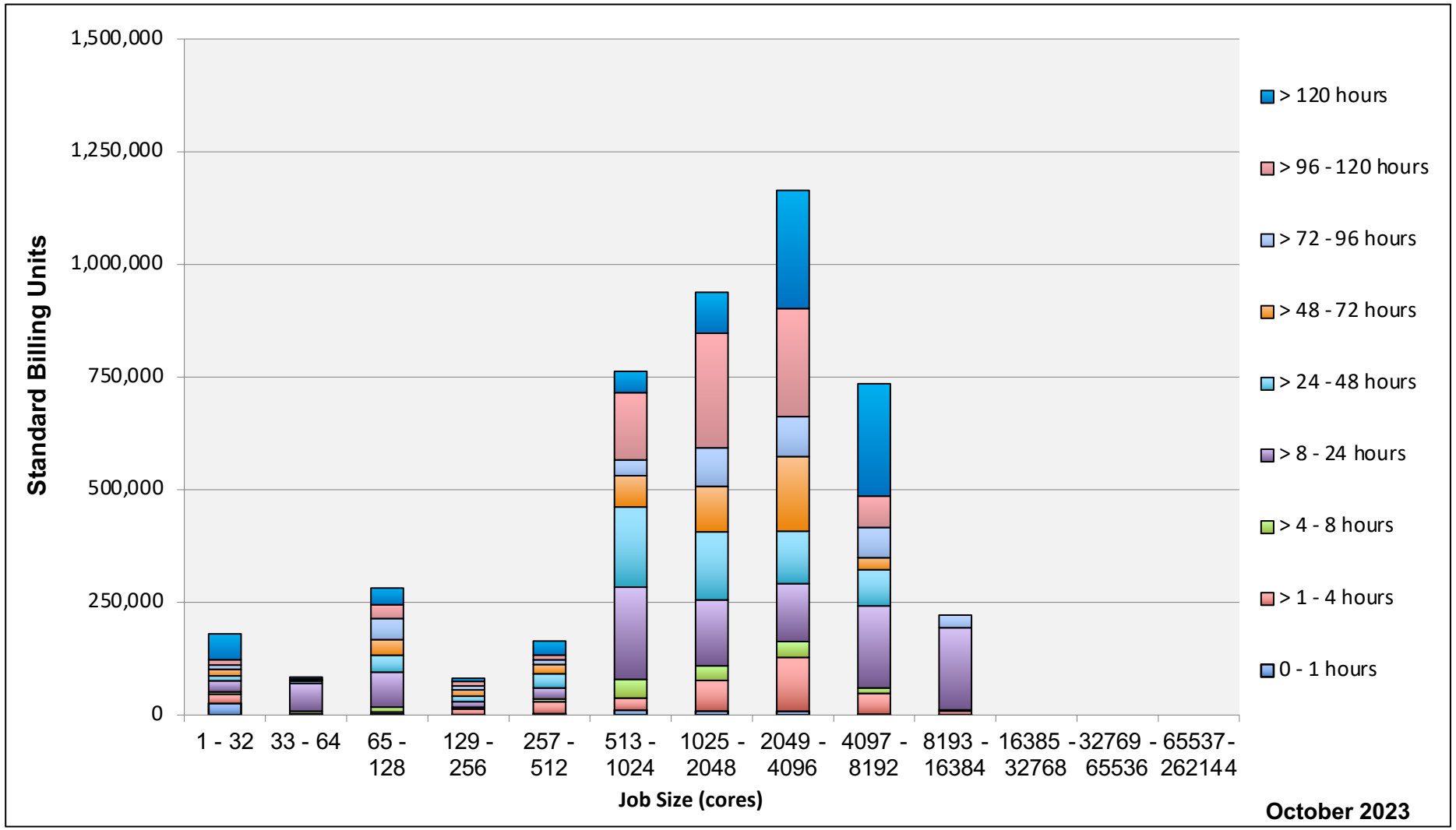
Pleiades: Monthly Utilization by Job Length



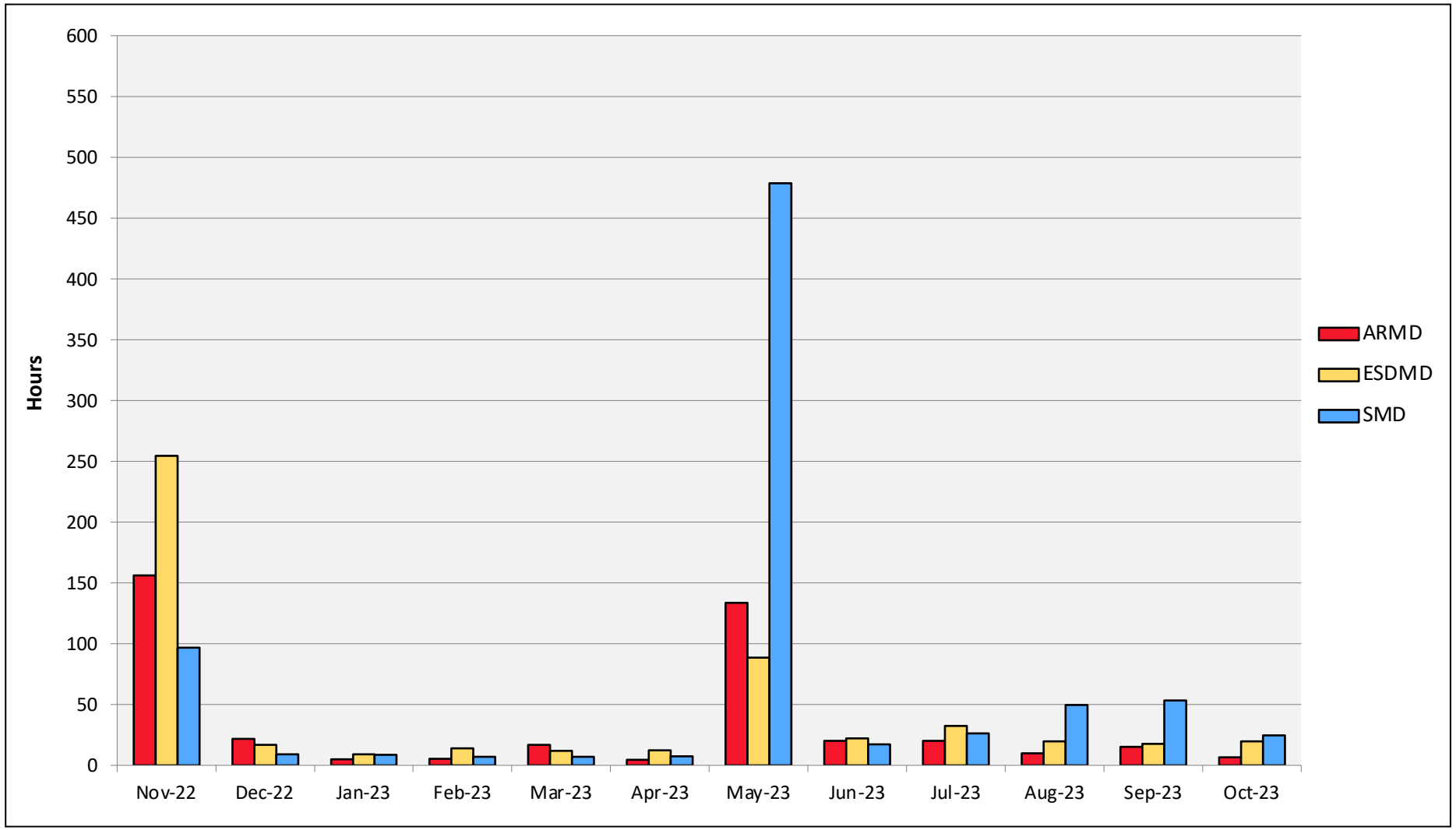
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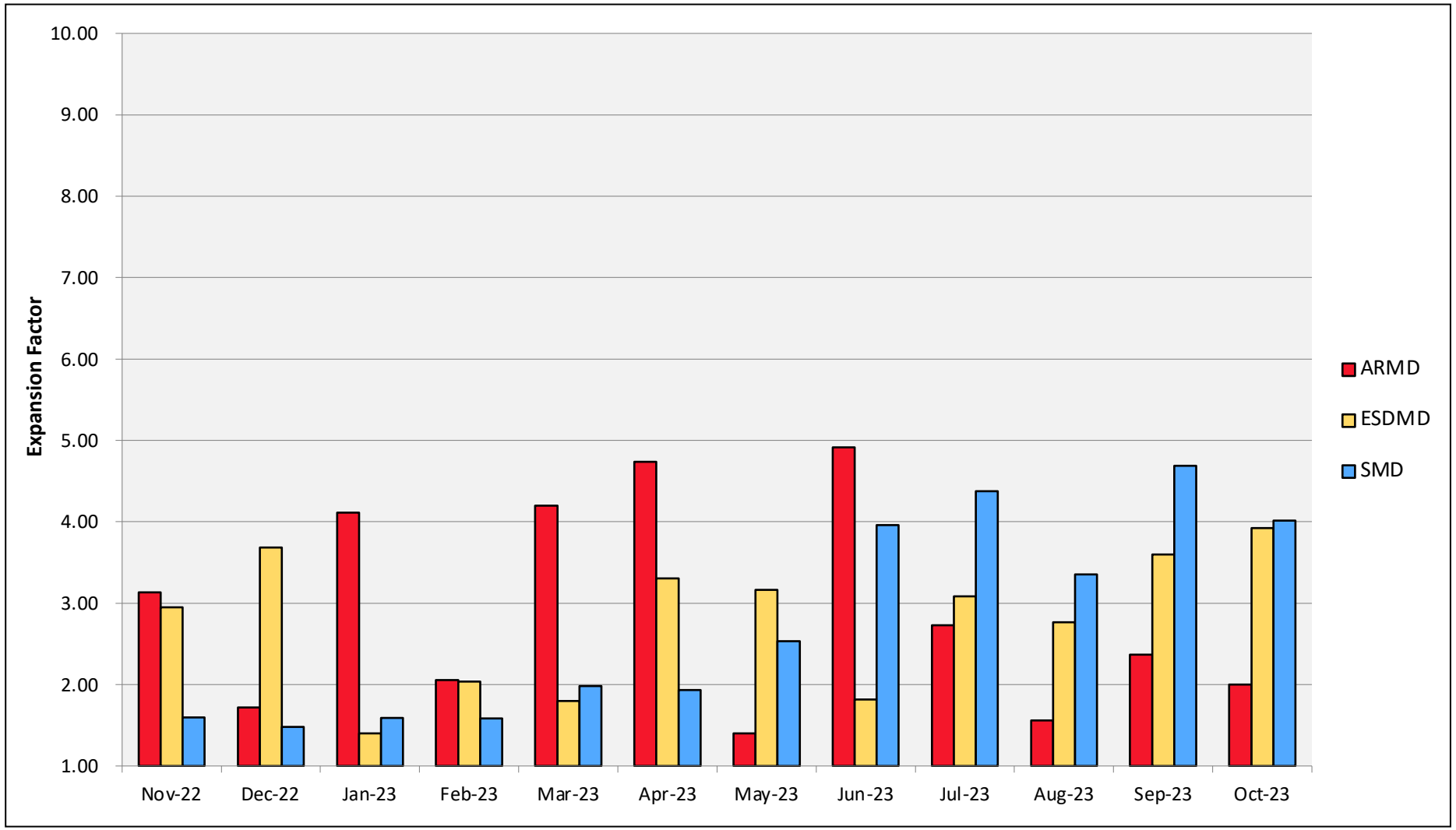
Pleiades: Monthly Utilization by Size and Length



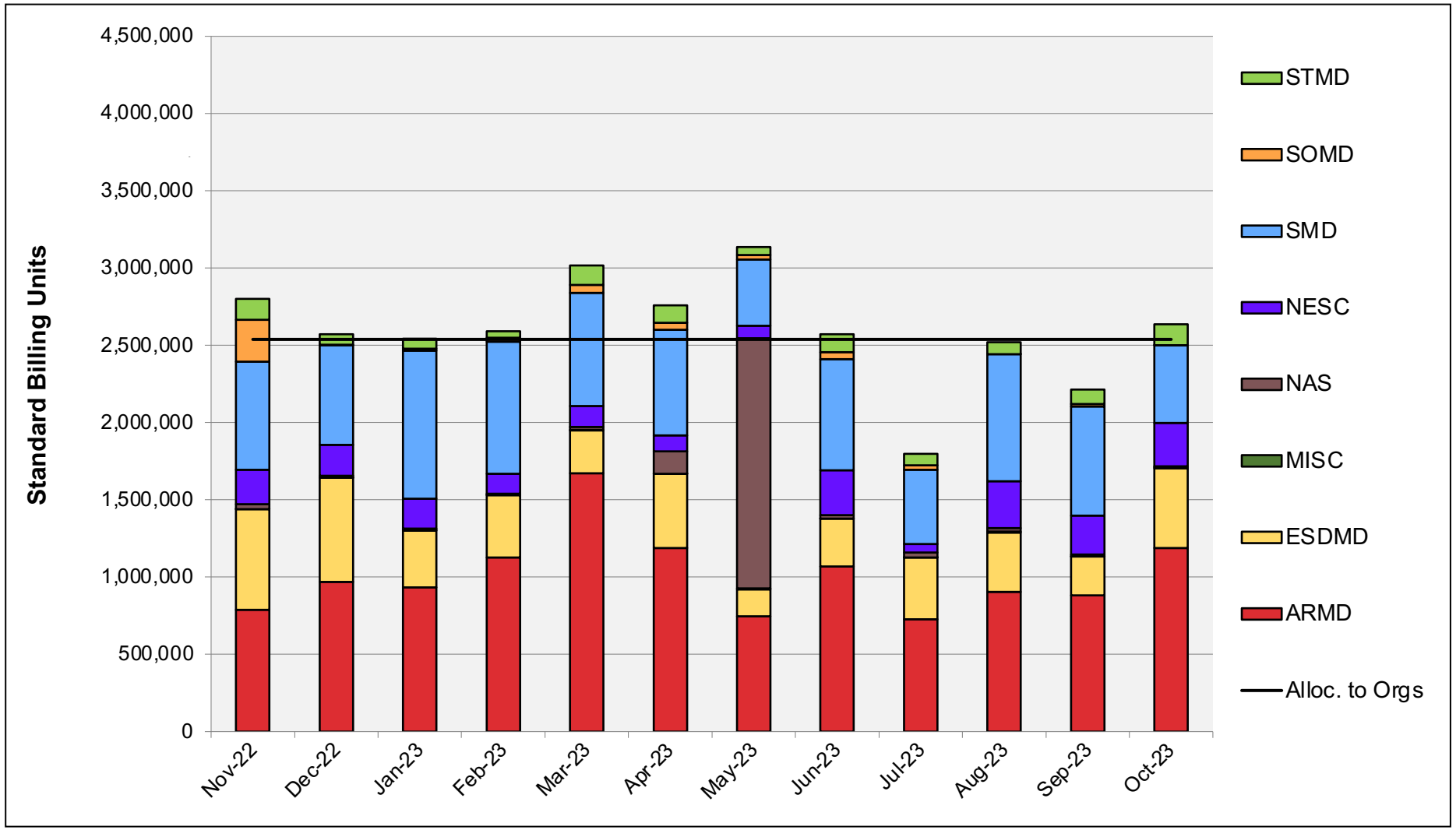
Pleiades: Average Time to Clear All Jobs



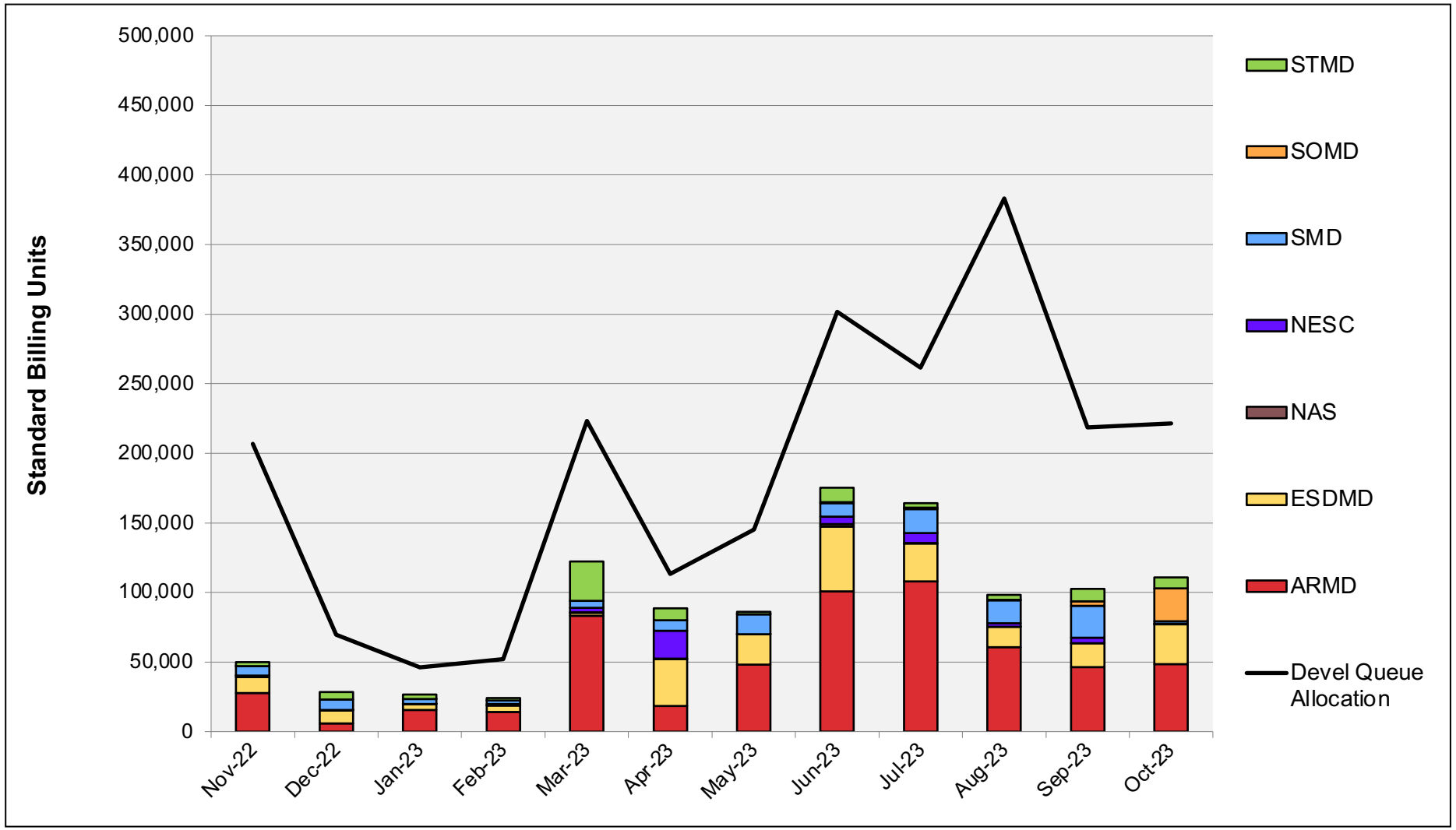
Pleiades: Average Expansion Factor



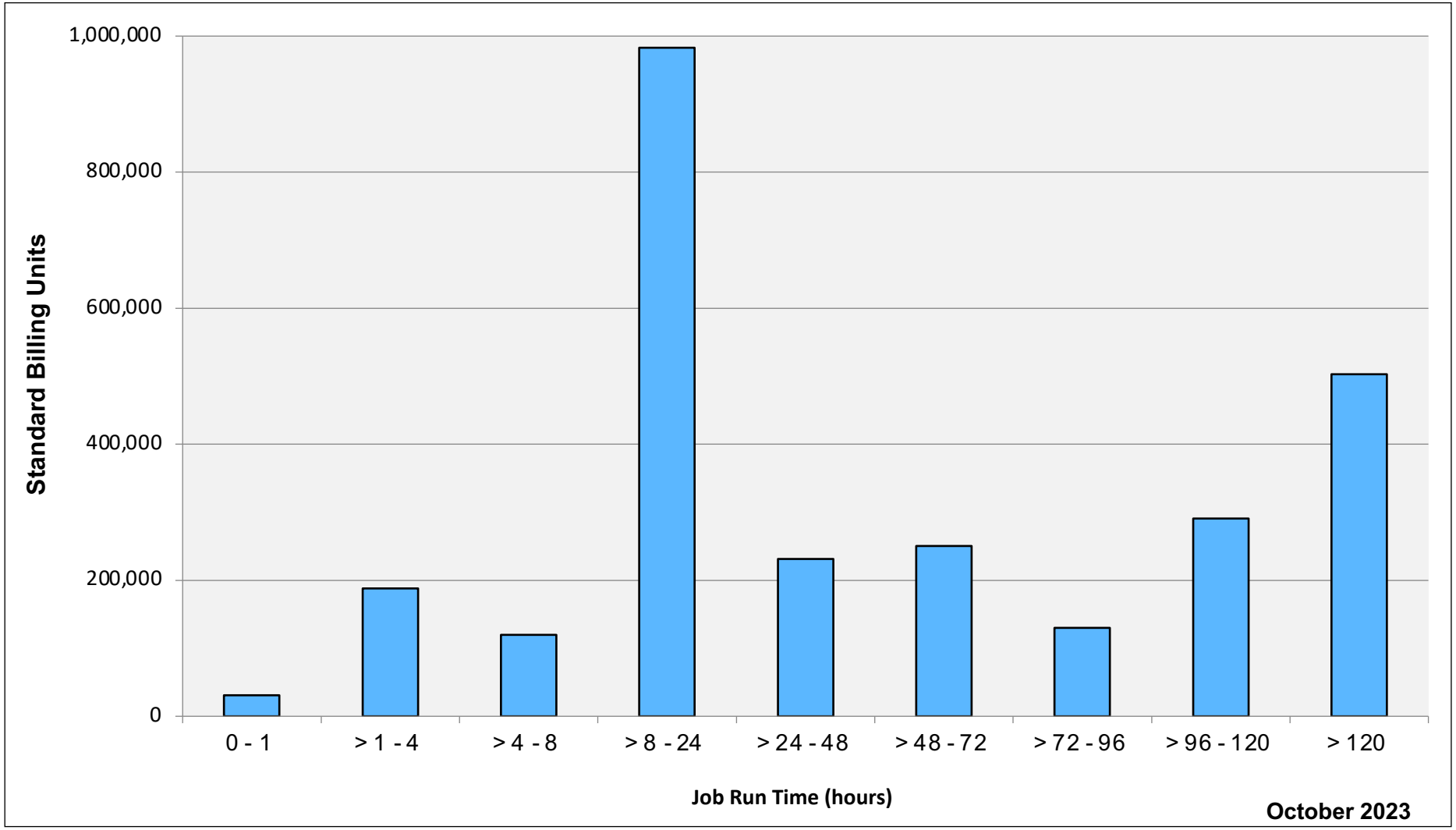
Electra: SBUs Reported, Normalized to 30-Day Month



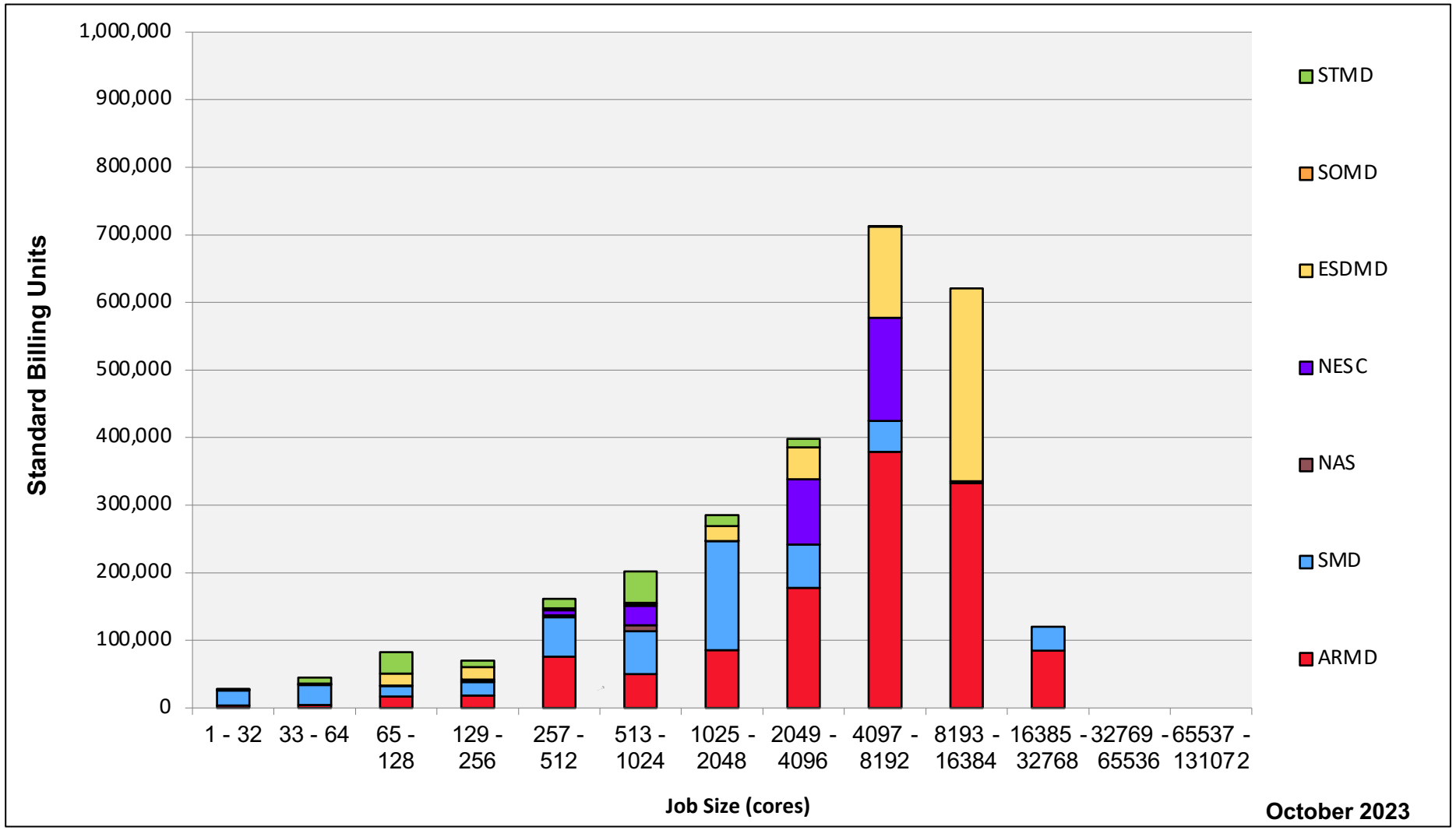
Electra: Devel Queue Utilization



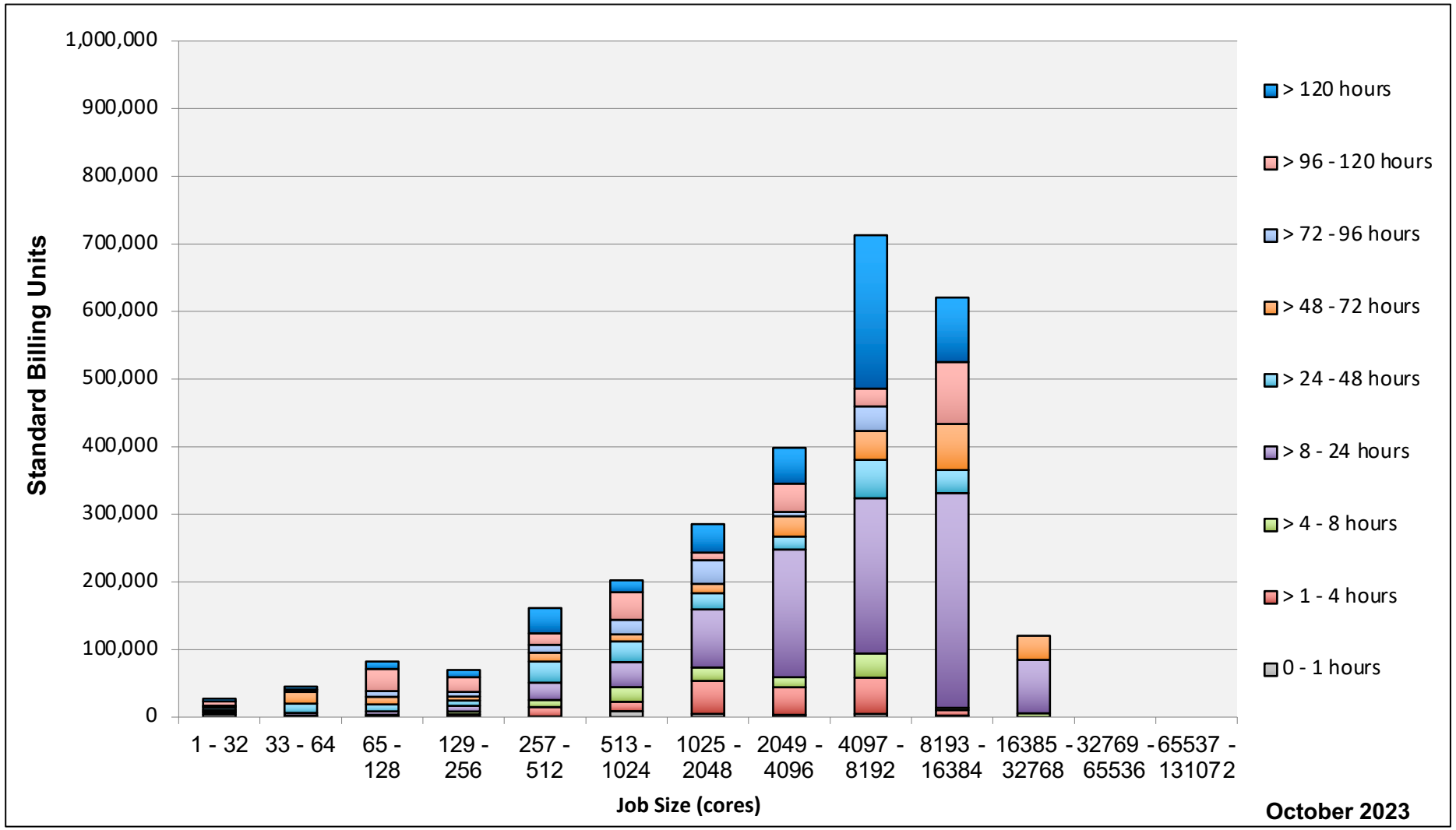
Electra: Monthly Utilization by Job Length



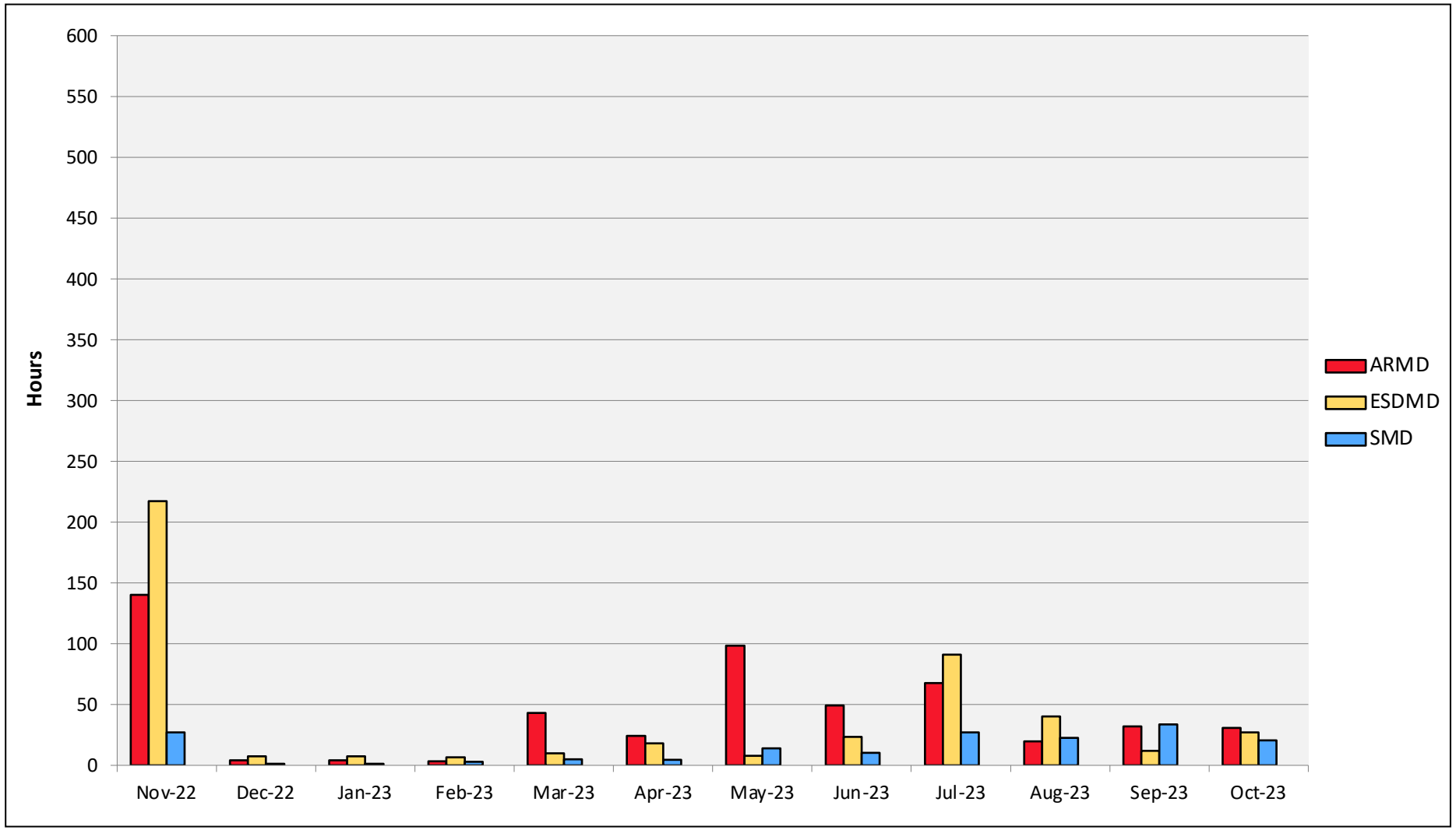
Electra: Monthly Utilization by Job Size



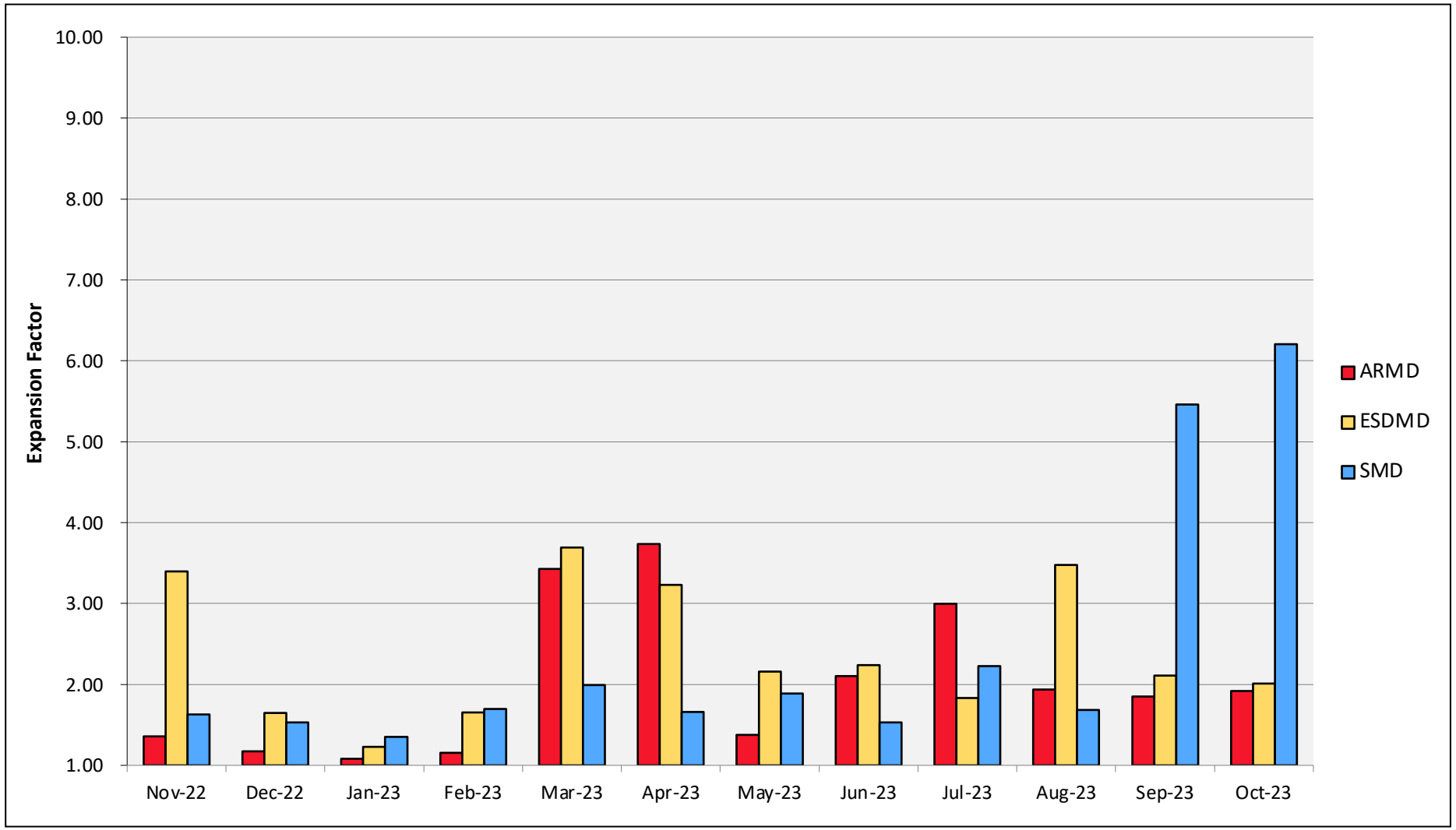
Electra: Monthly Utilization by Size and Length



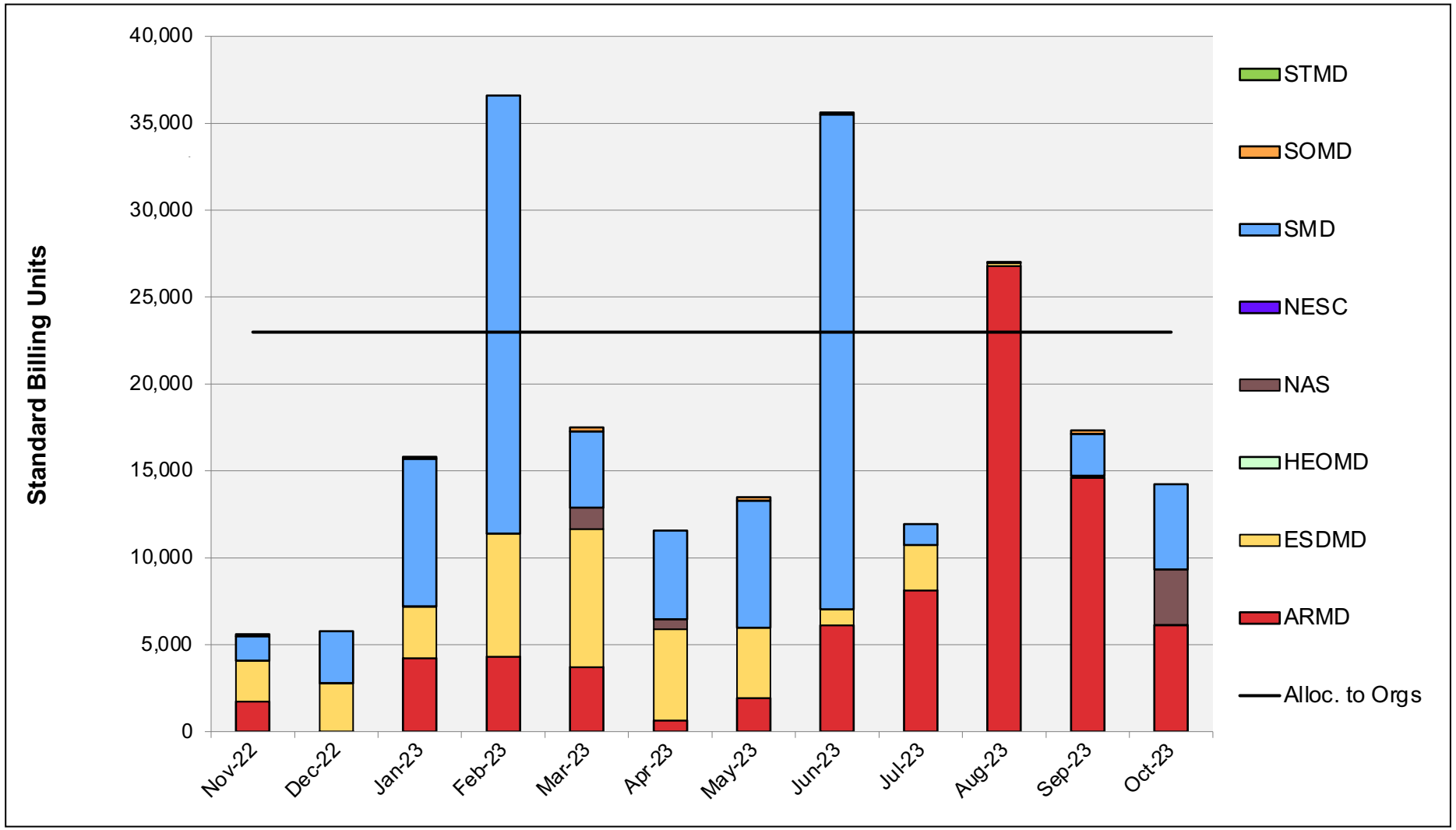
Electra: Average Time to Clear All Jobs



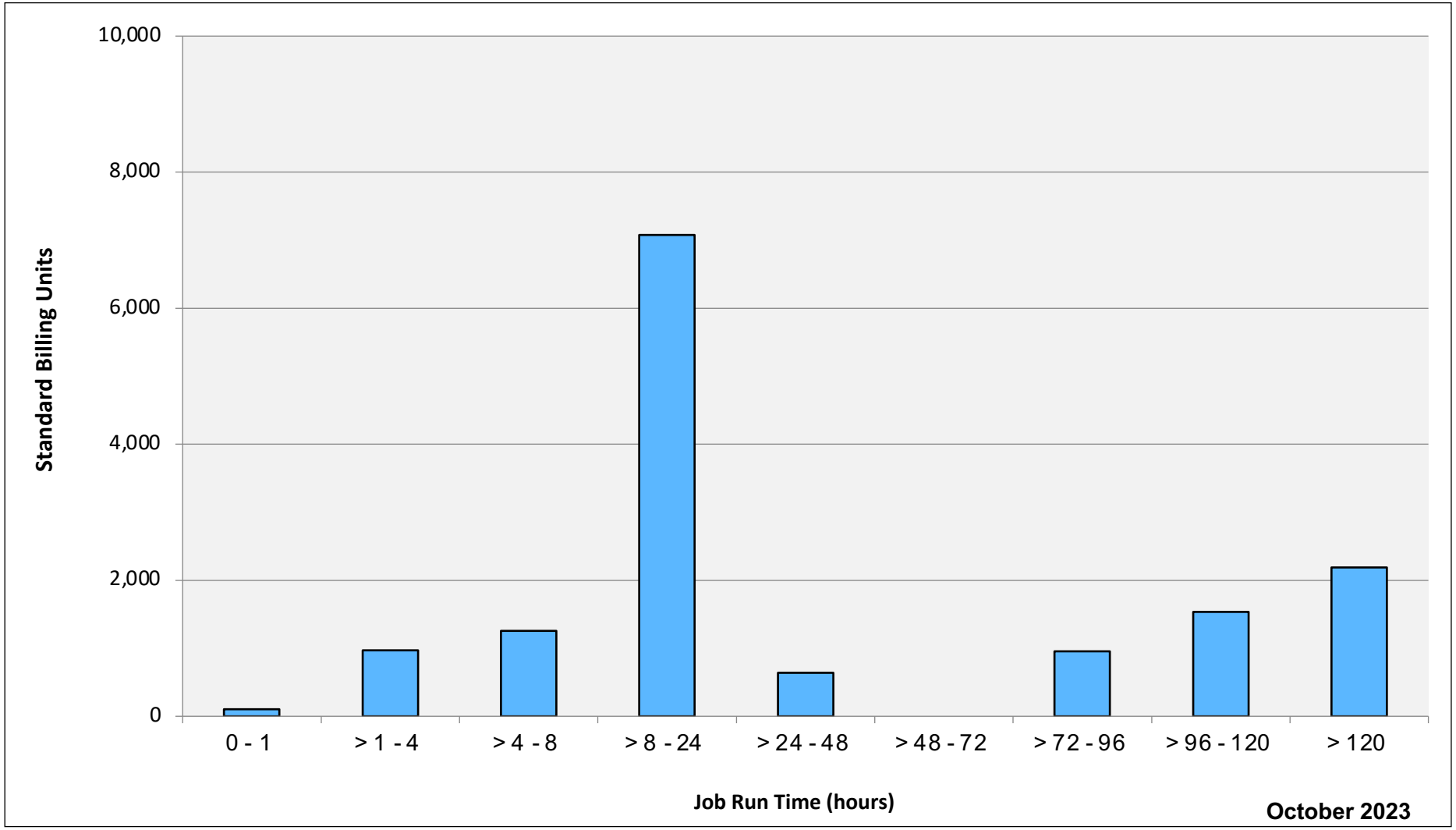
Electra: Average Expansion Factor



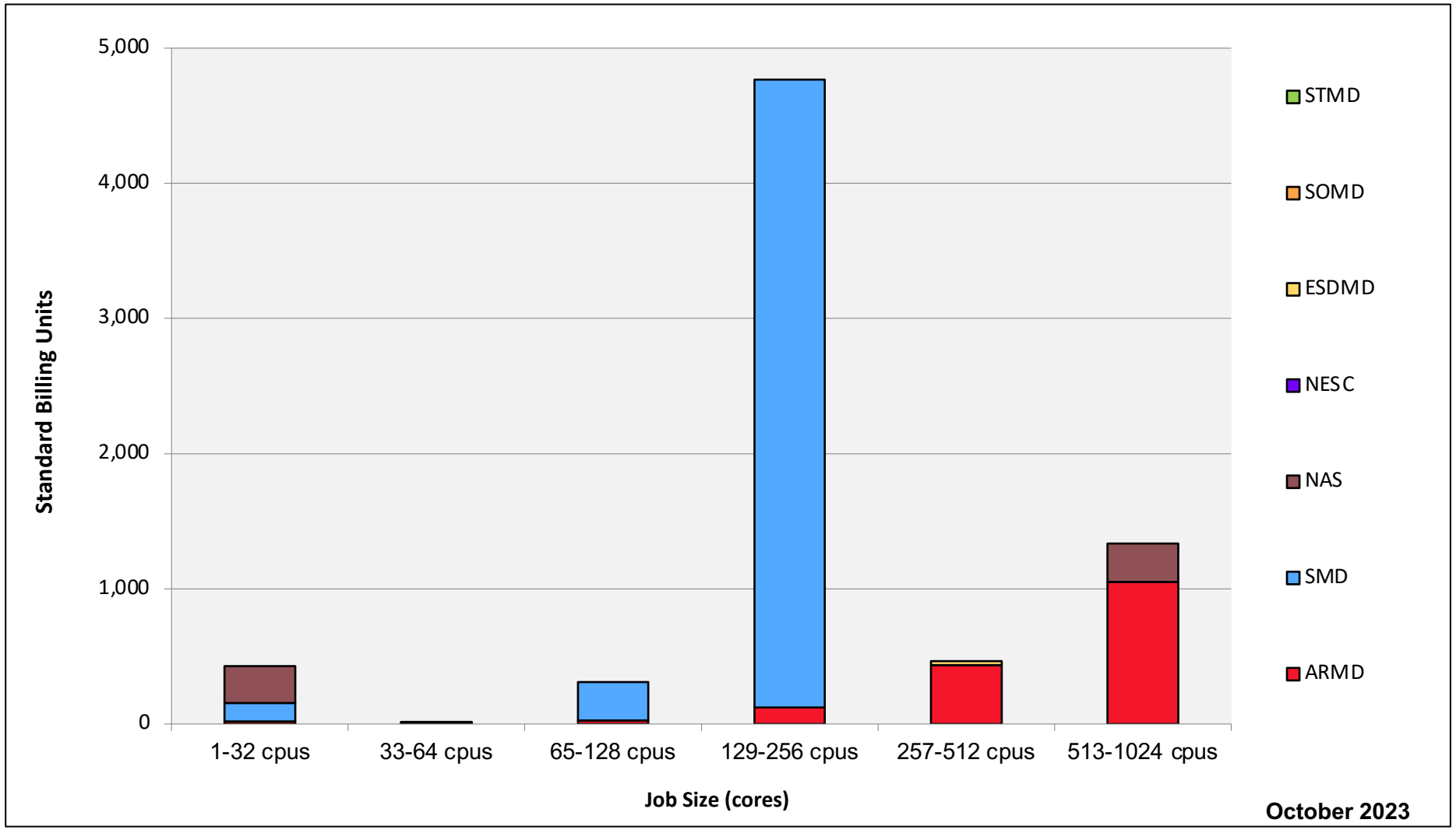
Endeavour: SBUs Reported, Normalized to 30-Day Month



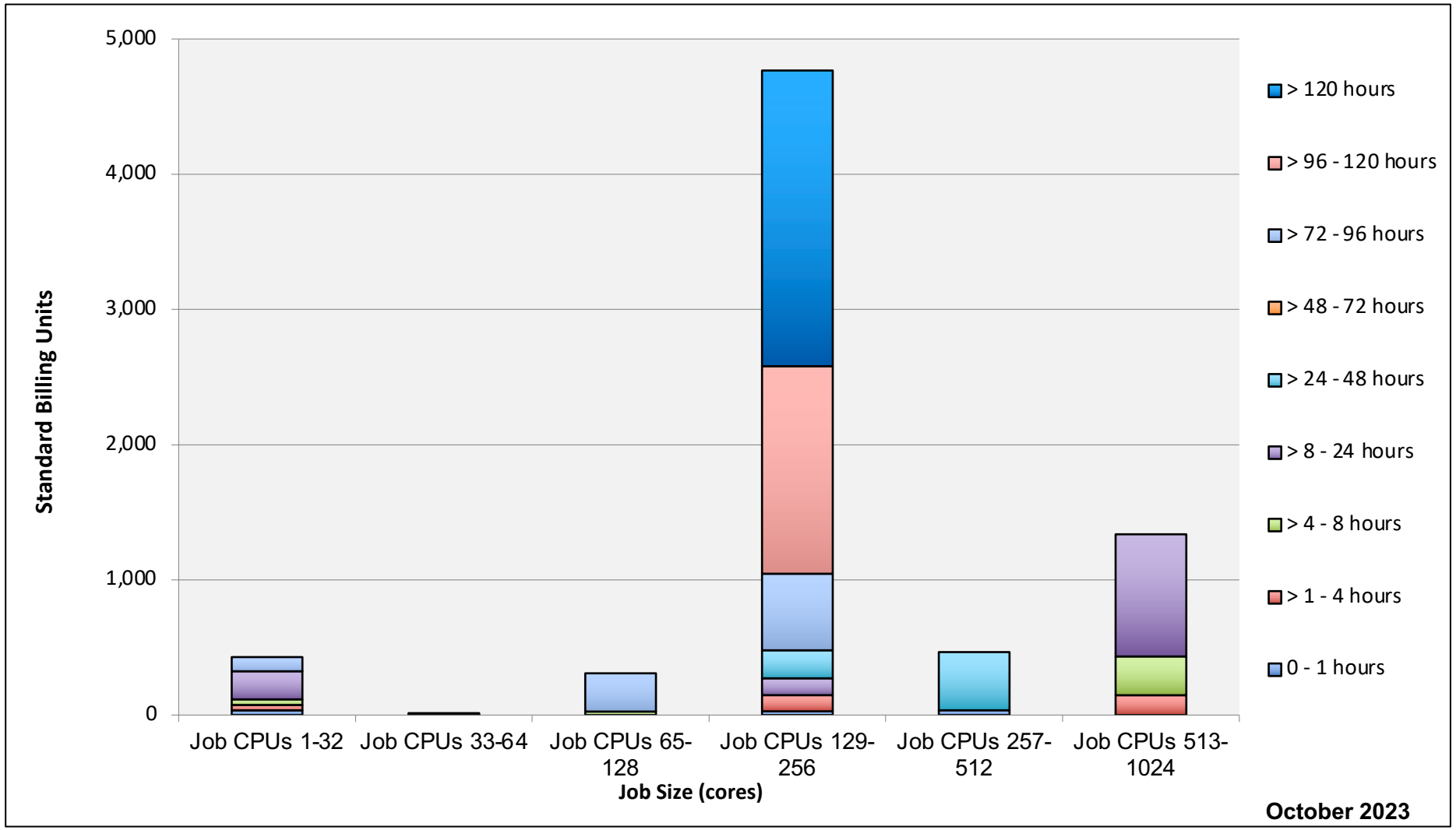
Endeavour: Monthly Utilization by Job Length



Endeavour: Monthly Utilization by Job Size



Endeavour: Monthly Utilization by Size and Length



Endeavour: Average Expansion Factor

