

National Aeronautics and Space Administration

High-End Computing Capability

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

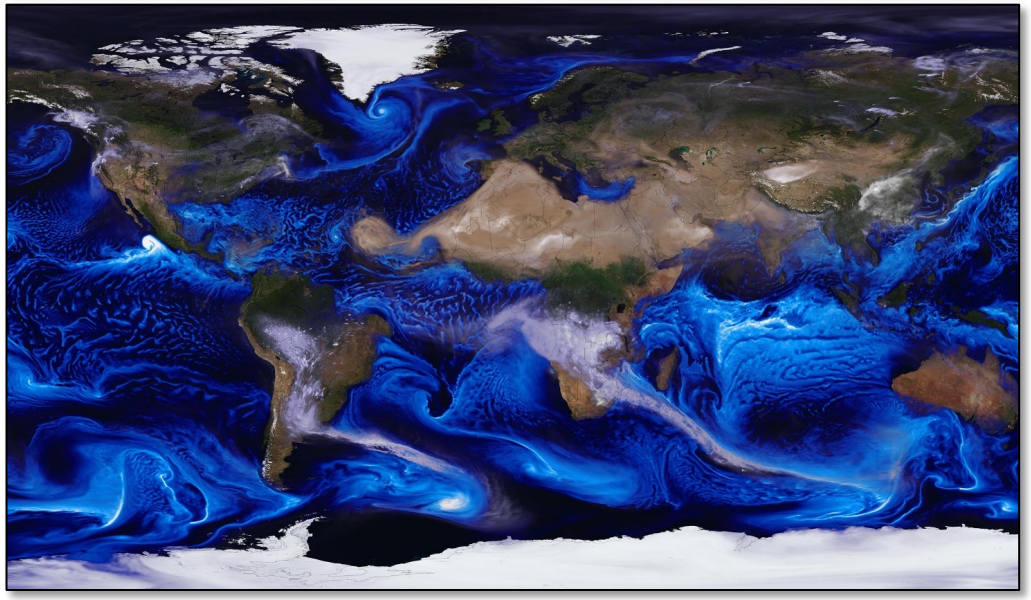
September 10, 2023

HECC Supercomputer Usage Sets New Normalized Record

- In August, the combined usage of HECC supercomputers set a new normalized record of 14,896,291 Standard Billing Units (SBUs*).
- The usage by 373 of NASA's science and engineering groups exceeded the previous record of 14,258,671 SBUs set in April 2023 by 637,620 SBUs.
- The record was achieved in great part by the Science Mission Directorate supporting many high-resolution simulations with the Goddard Earth Observing System (GEOS) for future observing system development. These simulations approach 1.5 kilometers globally, and focus has been placed on extreme events and storm-scale processes in these simulations.
- Usage of Aitken, Pleaides, Electra, and Endeavour contributed to this record. The new record is greatly attributed to the Aitken Rome nodes, with 128 cores per node.
- The top 10 projects' usage ranged between 256,712 and 2,086,093 SBUs, and together accounted for over 49% of the total usage.
- The HECC Project continues to evaluate and plan resources to address the future requirements of NASA's users.

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

IMPACT: The increased capacity of HECC systems and expert support to help users optimize their run capacities provide mission directorates with more resources to accomplish their goals and objectives.



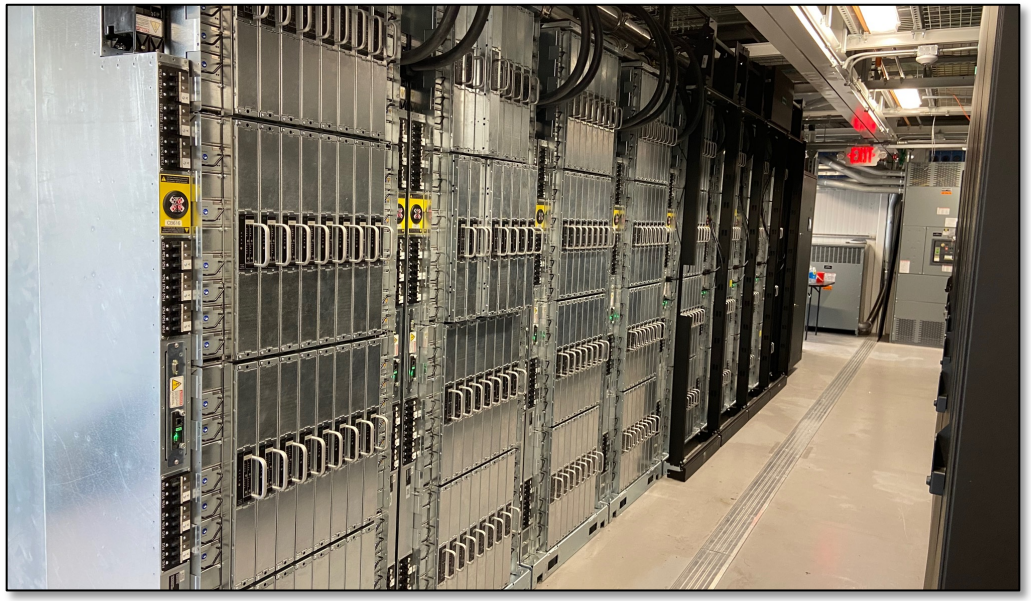
Snapshot of forecasted aerosol optical depth from the GEOS model at 12-kilometer horizontal resolution, with blue plumes representing sea salt; white, carbon; and brown, dust. Features visible are dust plumes streaming from the Sahara into the Atlantic, carbon emissions from fires in Africa, and cyclones traced by sea salt in the Pacific.
William Putman, NASA/Goddard

HECC Completes Annual Shutdown Tasks

As part of the HECC annual shutdown completed in July, the Computer Systems and Services (CSS) team systems engineers performed several important tasks:

- Updated the HPE Performance Cluster Manager (HPCM) to v1.9 for non-Rome nodes and the Lou archive storage cluster.
  - HPCM is HECC's provisioning management tool. It is foundational to the management of the cluster environment and takes a significant effort to update. During the shutdown, staff took the opportunity to update the service nodes, compute nodes, and archive administrative servers to the latest version of HPCM.
- Updated firmware for all the different components in the HECC cluster environment.
  - This ongoing task is done piecemeal throughout the year, and updating firmware on all systems at the same time is rarely possible. Doing so during the annual shutdown significantly reduced the total administrative time for the required tasks, which reduced the total downtime for users.
- Returned offline Pleiades Ivy Bridge compute nodes back into service.
  - Several hundred Ivy Bridge nodes were offline during the June 2023 migration to Red Hat Enterprise Linux 8-based Tri-Lab Operating System Stack Version 4 (TOSS 4) due to node discovery issues related to the conversion from the previous tool to HPCM. During the shutdown, the CSS team resolved the issue and brought these nodes back online for users.

IMPACT: These complex tasks performed simultaneously across the HECC cluster environment were done during the annual shutdown to avoid impacting users, and will significantly reduce administrative time for upcoming tasks.

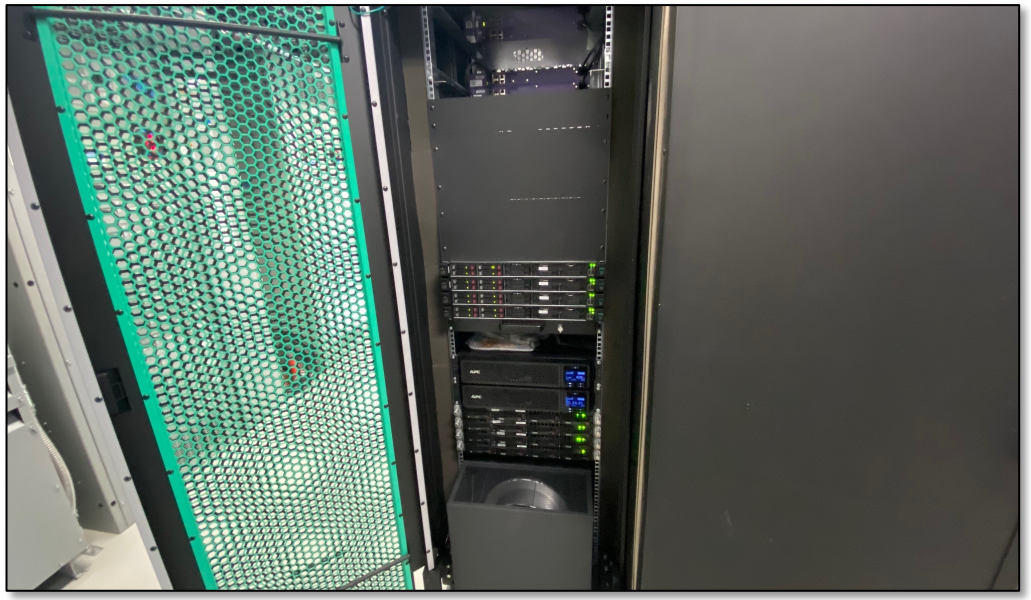


The Aitken supercomputer at NASA's Ames Research Center was updated during HECC annual shutdown. *Chris Tanner, NASA/Ames*

Electra Skylake Nodes Get Cooling Upgrade

- HECC facility engineers installed a new in-rack air conditioning unit in the Electra Skylake I/O rack residing in the Modular Supercomputing Facility (MSF) R&D088 module. The new air conditioning unit will improve the resiliency of the I/O rack's IT equipment on hot days.
- The new in-rack air conditioning unit has a 3-ton cooling capacity, with the evaporator occupying just the bottom 10 rack units of the I/O rack and the condenser installed on the module exterior. Power consumption is only 3 kilowatts.
- The in-rack unit installation is the result of a root cause analysis on unplanned outages, which determined that supplemental cooling closely coupled to the I/O rack's eight Electra Skylake rack leaders would provide cooling redundancy on hot days.
  - In September 2022, the Electra Skylake compute nodes experienced an unplanned outage after three rack leaders powered off due to the shutdown of the existing computer room air conditioning (CRAC) unit in the MSF after multiple days over 100°F.
  - The existing CRAC unit is responsible for cooling all of the module interior air and was the sole provider of cooling for the rack leaders in Electra Skylake I/O rack.
- The new in-rack air conditioning unit provides resiliency on hot days, improving compute availability in an energy efficient manner.

IMPACT: The additional cooling capacity to the Electra Skylake compute nodes will reduce unplanned outages on high-temperature days and maintain the availability of computing resources to the HECC user community.

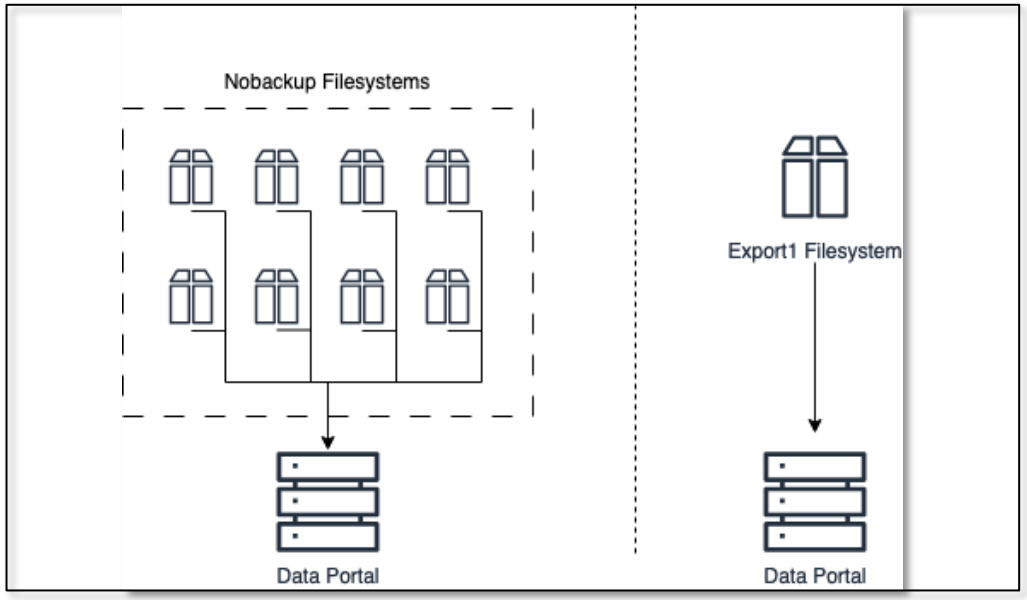


The in-rack air conditioning unit installed at the bottom of the Electra Skylake I/O rack provides cooling to the Skylake rack leaders directly above. *Chris Tanner, NASA/Ames*

Migration of HECC Data Portal's Datasets Results in Improved Availability for Users

- The Data Portal team worked with the Systems team to successfully transfer all published data in the HECC Data Portal to a dedicated filesystem called "export1."
- This effort included:
  - The teams migrated more than 6 petabytes of data spread across 15 datasets.
  - They configured the new export1 system as a read-only filesystem to facilitate data dissemination.
  - Disallowing active writes from compute jobs now results in enhanced performance of the export stack, reducing the potential for outages or workload-related impacts on the Data Portal.
- Previously, the Data Portal exported public datasets across eight different filesystems in the NAS secure enclave.
  - The stack that exports all the data relied on all datasets being available at all times. When one or more nobackup filesystem became unavailable, or experienced an unusually high load, a cascading failure would result in the Data Portal being unable to serve data.
- A new data management plan was created to govern how datasets are stored on the new filesystem. This allows multiple teams to move and release datasets that meet security and data permission requirements. Additionally, MD5 hash files are created in each directory to allow users to verify values of files after downloading them to their systems from the Data Portal.

IMPACT: With the transition to a single filesystem, the HECC Data Portal experiences significantly less downtime and is able to provide users with a more stable experience for accessing data provided by users and collaborators.



Top-level diagram detailing the storage of HECC Data Portal data before (left) and after migration.

New Verification and Tracking Process for Patching HECC Tools Team Hosts

- The HECC Tools and Engineering Systems Services (ESS) teams worked together to improve the overall process and stability for applying security patches to Tools host systems, implemented new processes for patch verification and tracking for 46 hosts, and established best practices for process efficiency.
- The Tools experts reduced the time and effort for the patching process from two weeks to three days. The team further reduced the time it takes to verify the hosts from 36 to 4 hours.
- The team implemented a tracking process to ensure all hosts are verified. The tracking process aids in reducing duplication efforts spent by the team. Further, the new process allows everyone to see who verified the host, issues, and completion status. A shared Excel spreadsheet is available to all team members to view real-time patching status.
- The team worked with ESS to establish best practice standards, such as: Rebooting hosts regardless of patching status to minimize point of failure; a standard method of communication that ensures essential staff availability, issue reporting, and status; evolving available ESS processes such as email notifications for status of promotion and reboot of all hosts, as well as user notification for necessary High Impact Production Patching (HIPP) host downtimes, such as Remedy; and process improvements for automating service restarts after reboot.
- The verification steps identified will allow the Tools team to automate this new process. These proactive steps will be implemented using Nagios monitoring and various scripting languages. Another benefit of implementing patching procedures in Nagios: it will allow alerts for Tools support for host and service issues.

IMPACT: The successful implementation of standard verification and new tracking procedures following security patching has significantly reduced the number of hours required to verify host systems supported by the HECC Tools team. The new process safeguards production and HIPP machines by tracking confirmation of successful patching of both development and staging hosts.

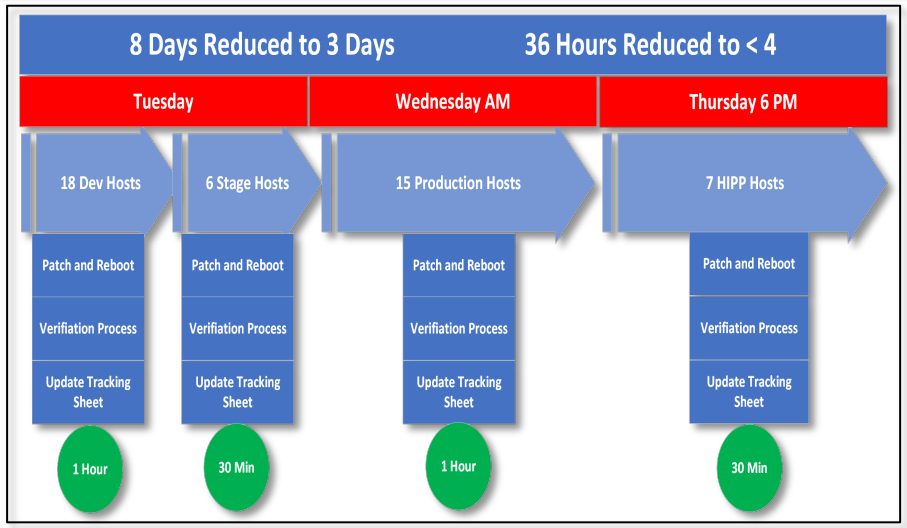
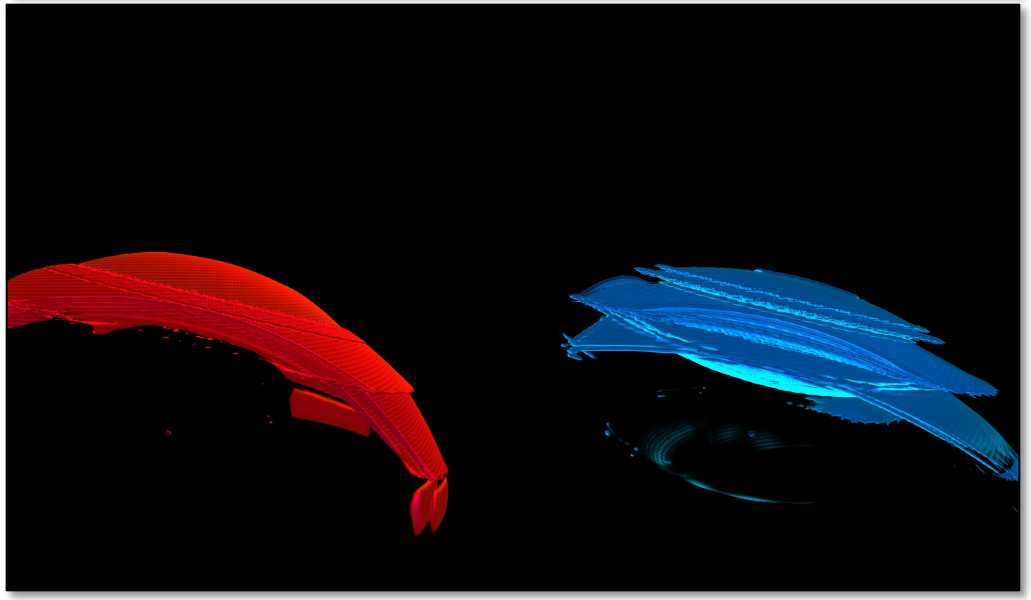


Chart showing the time savings attained from the new weekly patching process, reducing the prior 8-day duration to 3 days for 46 hosts. The new process requires 1 hour for development and production hosts and 30 minutes for staging and HIPP hosts, reducing the total effort from 36 to less than 4 hours.

More Performance Improvements to specFEM3D Code for USGS Earthquake Simulations

- HECC's Visualization and Data Analysis team further improved the performance of the open source "specFEM3D" code used by the U.S. Geological Survey (USGS) to simulate earthquakes.
- The specFEM3D developers had added OpenMP to the code, but the implementation was less than ideal.
  - Parallelized just a few loops.
  - Used "atomic operations" to break dependencies, which has the drawback of getting (very slightly) different answers every time the code is run, and also experiences thrashing at high thread counts.
  - As is, the code runs about 6 times faster with 16 threads, compared to the non-OpenMP version when run on the Pleiades supercomputer.
- The Vis team's improvements include: Parallelized additional loops; removed the atomic operations, and broke the dependencies using a more sophisticated scheme.
- These techniques significantly improved the specFEM3D results.
  - Now always gets the same answer, regardless of thread count.
  - Runs about 10 times faster than the non-OpenMP version on 16 threads, a 65% improvement over the original.
  - Obtained more than a order of magnitude higher-resolution than the usual USGS run, and in less time.

IMPACT: USGS users can do more, higher-resolution, and faster earthquake modeling with HECC's Visualization and Data Analysis team's code optimizations of specFEM3D.

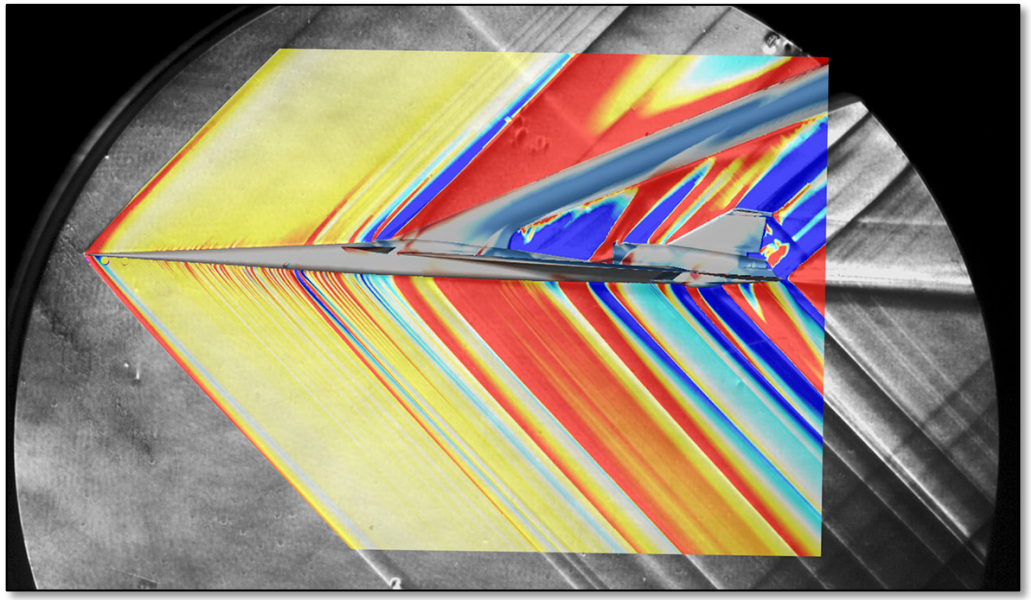


High-resolution simulation of seismic waves from a deep earthquake interacting with a subducting tectonic slab (not shown). The idealized earthquake produces only pressure waves (red), but shear waves (blue) are produced by "mode conversion" at the slab boundaries where material properties change abruptly. Analyzing the converted waves detected by seismometers on the surface allows seismologists to infer subsurface structures using tomographic methods. *Chris Henze, NASA/Ames*

Advancing NASA Software for Sonic Boom Prediction*

- Teams of researchers at NASA Ames are using the agency's Cart3D and Launch Ascent and Vehicle Aerodynamics (LAVA) flow solvers to help create flight planning software for the agency's X-59 low-boom supersonic aircraft, running thousands of high-fidelity computational fluid dynamics (CFD) simulations on HECC systems.
- The X-59 must be able to fly at supersonic speeds without creating an objectionable sonic boom on the ground and fly at a target loudness level across a wide range of conditions. To ensure the aircraft performs as required, the flight planning software will inform pilots how to fly the aircraft to achieve desired loudness levels for testing.
  - The simulations help identify features on the aircraft that contribute to the sonic boom pressure signal and predict loudness levels experienced on the ground.
  - To minimize the cost of developing the flight software, the Ames researchers are working to improve their analysis tools, increasing the speed of individual calculations, and furthering understanding of low-boom aircraft physics.
  - The methods developed by the LAVA team reduced the computational resources required to get a high-fidelity CFD solution by a factor of at least 2—leading to significant cost savings over the large number of cases required to develop the X-59 sonic boom prediction database.

IMPACT: With construction of the X-59 aircraft well underway, the improvements made to NASA's LAVA and Cart3D frameworks are helping to generate the sonic boom prediction databases needed by mission engineers to develop advanced flight planning software.



A schlieren image from a wind-tunnel test of the X-59 model is compared with a simulation of the test. *Marian Nemec, Michael Aftosmis,* NASA/Ames

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

Multiphase SLS Launch Environment Simulations*

- Engineers at NASA Marshall utilized HECC supercomputers to perform simulations of the Space Launch System ignition sequence prior to the Artemis I launch in November 2022. During launch, the SLS propulsion system generates intense acoustics and other powerful waves, such as ignition overpressure (IOP), which, if left unmitigated, have the potential to damage the vehicle and put the crew and mission at risk.
- The Marshall team used the Loci/STREAM-Volume of Fluid multiphase computational fluid dynamics (CFD) solver to simulate the SLS ignition sequence—from the activation of the SLS main engine and solid rocket boosters to just prior to liftoff—including the water-based IOP sound suppression system of the launch pad at NASA Kennedy.
- The simulations were conducted on meshes up to hundreds of millions of cells, on thousands of processors, for weeks at a time, and generated terabytes of data. The results provided a deeper understanding of the physics that occur during launch, which was largely unknown before the uncrewed Artemis I launch, due to differences from previous programs.
- Post-launch comparisons of gathered Artemis flight data against the CFD simulation results help to validate these computational tools, which can be applied to future missions and launch vehicles, such as the more powerful Block 1B configurations, with confidence.

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

IMPACT: Simulations like these provide insights into the complex launch environment, especially in areas that are obstructed from measurement tools, in addition to helping interpret flight data and identify safety concerns.



Visualization of the SLS's RS-25 rocket plume-water interaction simulation.
Travis Rivord, NASA/Marshall; Patrick Moran, NASA/Ames

Papers

- "**Propagation of a Realistic Magnetar Jet through a Binary Neutron Star Merger Medium and Implications for Short Gamma-Ray Bursts**," G. Soares, et al., *The Astrophysical Journal*, vol. 953, no. 1, August 3, 2023. *
  https://iopscience.iop.org/article/10.3847/1538-4357/ace167/meta
- "**Radial Distribution of Distant Trans-Neptunian Objects Points to Sun's Formation in a Stellar Cluster**," D. Nesvorny, et al., *Icarus*, vol. 406, published online August 4, 2023. *
  https://www.sciencedirect.com/science/article/abs/pii/S0019103523003159
- "**Impact Rates in the Outer Solar System**," D. Nesvorny, et al., *The Planetary Science Journal*, vol. 4, no. 8, August 8, 2023. *
  https://iopscience.iop.org/article/10.3847/PSJ/ace8ff/meta
- "**Asymptotic Scaling Relations for Rotating Spherical Convection with Strong Zonal Flows**," J. Nicoski, et al., arXiv:2308.05174 [physics.flu-dyn], August 9, 2023. *
  https://arxiv.org/abs/2308.05174
- "**Identification of the Top TESS Objects of Interest for Atmospheric Characterization of Transiting Exoplanets with JWST**," B. Hord, et al., arXiv:2308.09617 [astro-ph.EP], August 18, 2023. *
  https://arxiv.org/abs/2308.09617
- "**Electron Acceleration and Heating During Magnetic Reconnection in the Earth's Quasi-parallel Bow Shock**," N. Bessho, et al., *The Astrophysical Journal*, vol. 945, no. 1, August 21, 2023. *
  https://iopscience.iop.org/article/10.3847/1538-4357/ace321/meta

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

Papers (cont.)

- "**Refining the Properties of the TOI-178 System with CHEOPS and TESS**," L. Delrez, A. Leleu, et al., arXiv:2308.11394 [astro-ph.EP], August 22, 2023. *
  https://arxiv.org/abs/2308.11394
- "**A Study of the Sensitivity of SAR Ocean Backscatter to Oil Slick Properties using an Electromagnetic Scattering Model**," S. Jaruwatanadilok, et al., *IEEE Transactions on Geoscience and Remote Sensing*, published online August 23, 2023. *
  https://ieeexplore.ieee.org/abstract/document/10227298
- "**TOI-332 b: A Super Dense Neptune Found Deep within the Neptunian Desert**," A. Osborn, et al., arXiv:2308.12137 [astro-ph.EP], August 23, 2023. *
  https://arxiv.org/abs/2308.12137
- "**Observations and Modeling of Unstable Proton and α Particle Velocity Distributions in Sub-Alfvénic Solar Wind at Parker Solar Probe Perihelia**," L. Ofman, et al., *The Astrophysical Journal*, vol. 954, no. 2, August 28, 2023. *
  https://iopscience.iop.org/article/10.3847/1538-4357/acea7e/meta
- "**TOI-4600 b and c: Two Long-Period Giant Planets Orbiting an Early K Dwarf**," I. Mireles, et al., *The Astrophysical Journal Letters*, vol. 954, no. 1, August 30, 2023. *
  https://iopscience.iop.org/article/10.3847/2041-8213/aceb69/meta
- "**A Super-Massive Neptune-sized Planet**," L. Naponiello, et al., *Nature*, published online August 30, 2023. *
  https://www.nature.com/articles/s41586-023-06499-2

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Presentations

- "**Enhancing Data Discoverability and Analysis for Understanding Space Radiation in Earth Environment with Radiation Data Portal**," Z. Watkins, et al., presented at the SHINE 2023 Workshop, Stowe, VT, August 7-13, 2023.
- "**Expanding the search for Earth-size Planets Orbiting Sun-like Stars by Compressing Image Data Onboard Space Telescopes**," J. Jenkins, presented at the 2023 Flash Memory Conference & Expo, Santa Clara, CA, August 8-10, 2023.
- **54th Meeting of the Solar Physics Division**, Minneapolis, MN, August 13-18, 2023.
  - "**3D Radiative MHD Modeling of Thermodynamical Coupling From Subsurface Layers of the Sun to Corona**," I. Kitiashvili, et al.
  - "**Utilizing Acoustic Power Maps and Machine Learning for Early Detection of Active Region Emergence**," S. Kasapis, et al.
  - "**Inferring Van Allen Radiation Belt Fluxes using Solar Dynamics Observatory Spike Data in Correlation with GOES-14 Measurements**," S. Kasapis, M. Shalaby, B. Thompson, J. Rodriguez, et al.
- "**Fluid-Structure Interaction Parachute Simulations For Interplanetary Missions**," F. Cadieux, presented at the Parachute FSI Workshop, Santa Ana, CA, August 15, 2023.
- **International Astronomical Union Symposium 365**, Yerevan, Armenia, August 21-25, 2023.
  - "**3D Radiative Hydrodynamic Modeling of Shallow Convection Zones of Main-Sequence Moderate-Mass Stars**," I. Kitiashvili.
  - "**Fine Structure of Differential Rotation and Meridional Flows in the Near-Surface Shear Layer of the Sun from 3D Radiative Hydrodynamics**," I. Kitiashvili.
  - "**Physical Properties of the Solar Atmosphere Derived from Comparison of Spectro-Polarimetric SDO/HMI Observables with 3D Radiative**," I. Kitiashvili.
  - "**Early Detection of Active Region Emergence in the Solar Interior Using Acoustic Power Maps and Machine Learning Data Analysis**," S. Kasapis.

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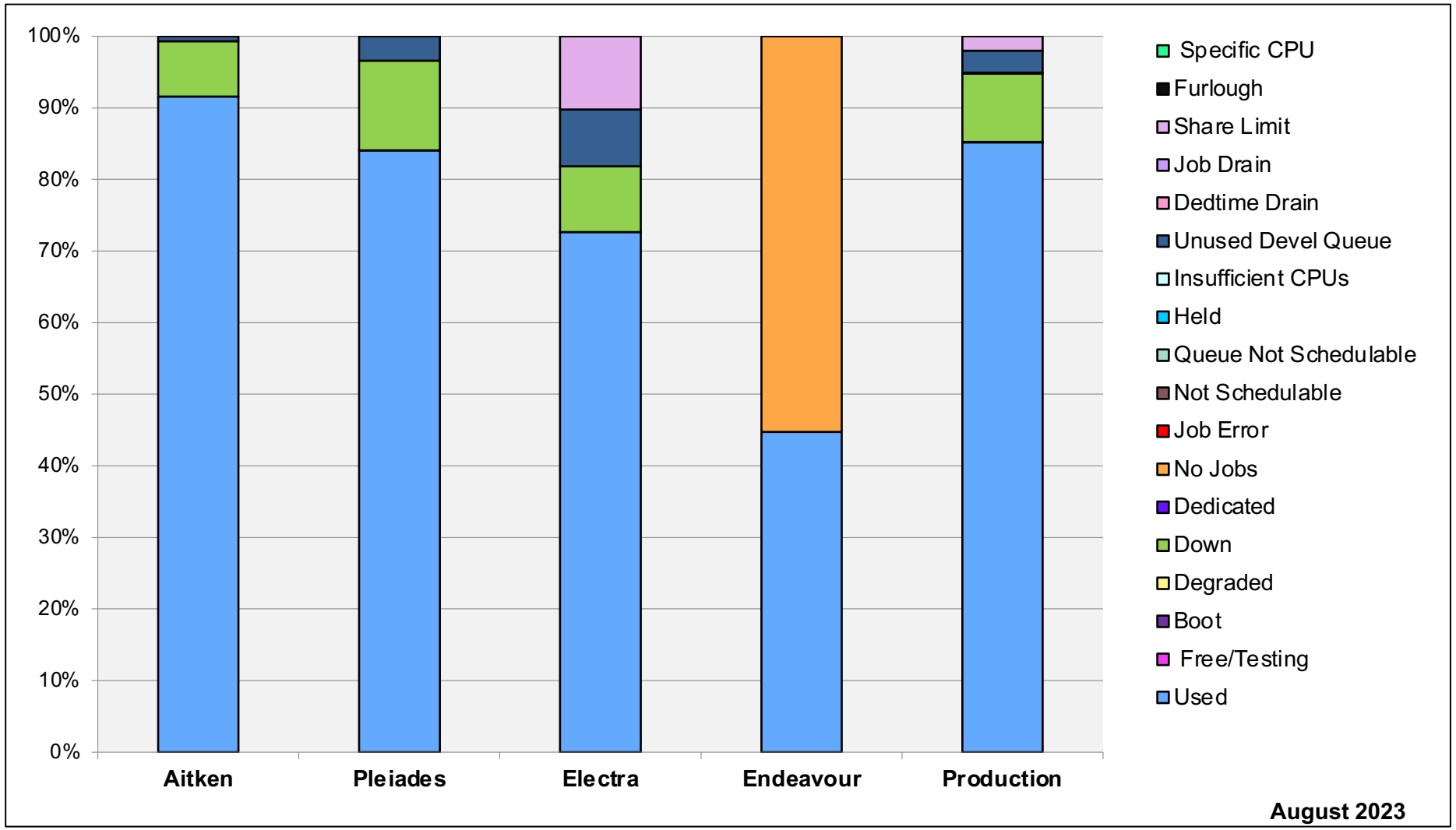
News and Events

- **NAS Summer Interns Share Science & Engineering Project Results**, *NAS Feature*, August 22, 2023—Students from around the U.S. and Canada wrapped up a three-month NASA summer internship opportunity at NAS, where each student was matched with NAS Division mentors with expertise in their fields of study.
  https://www.nas.nasa.gov/pubs/stories/2023/news_08-22-2023_summer_interns.html
- **Study Reveals Compounding Climate Risks at Two Degrees of Warming**, *NASA Ames Feature*, August 10, 2023—A NASA-led study showed that if global temperatures keep rising and reach 2 degrees Celsius above pre-industrial levels, people worldwide could face multiple impacts of climate change simultaneously.
  https://www.nasa.gov/feature/ames/nasa-study-reveals-compounding-climate-risks-at-two-degrees-of-warming/
- **Shining a Light on the Sun's Magnetic Field**, *NAS Feature*, August 7, 2023—Researchers at Northwestern University ran simulations of the Sun and other stars on the Pleiades cluster at the NASA Advanced Supercomputing facility and made some discoveries that help answer questions about how magnetic fields develop and travel to the surface.
  https://www.nas.nasa.gov/pubs/stories/2023/feature_sun_magnetic_field.html
- **Sea Surface Currents and Salinity Near the Maritime Continent**, NASA Global Modeling and Assimilation Office, August 1, 2023—NASA High-End Computing resources, including those at the NAS facility, enabled a modeling study of the Indonesian Throughflow, the only low-latitude gateway for export of large amounts of heat and freshwater from the Pacific to the Indian Ocean.
  https://gmao.gsfc.nasa.gov/research/science_snapshots/2023/sea-surface.php

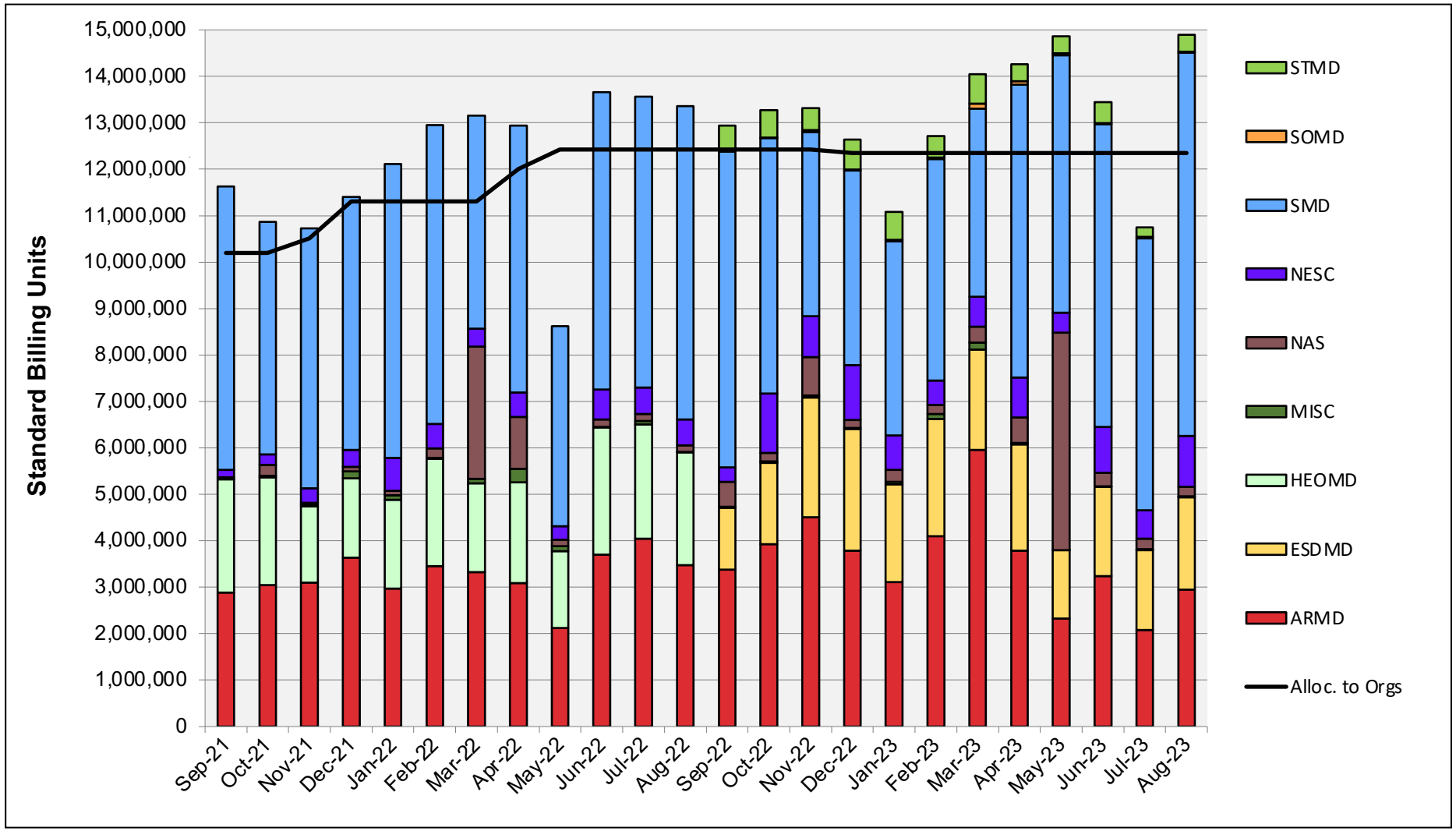
News and Events: Social Media

- **NAS Feature: Shining a Light on the Sun's Magnetic Field**
  - NASA Supercomputing: Facebook ~1,350 users reached, 20 reactions, 6 shares; X 774 views, 4 reposts, 9 likes.
  - NAS Division: X 318 views, 1 reposts, 1 quote, 4 likes.

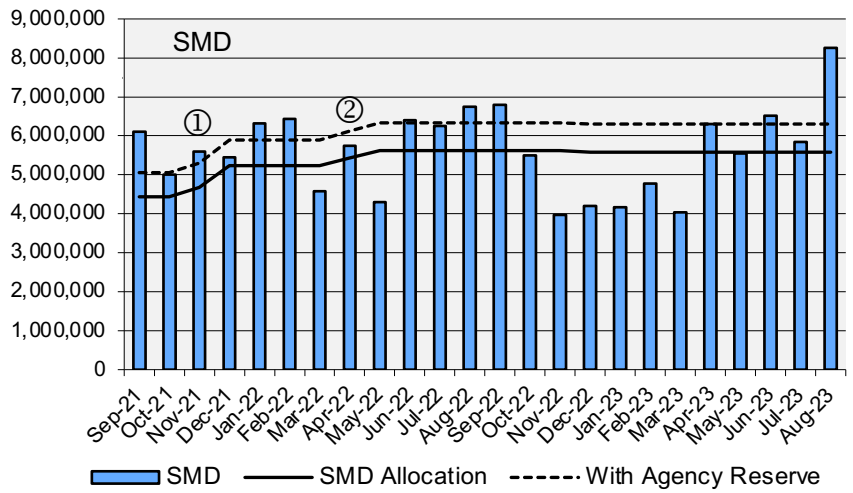
HECC Utilization

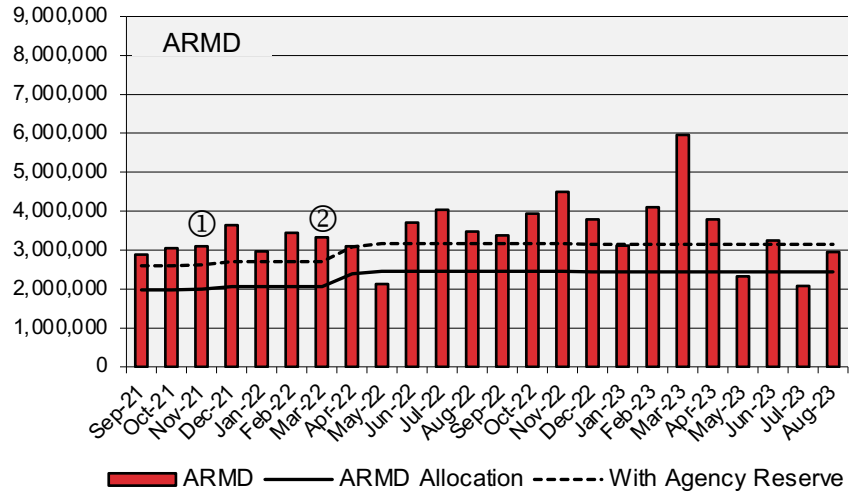


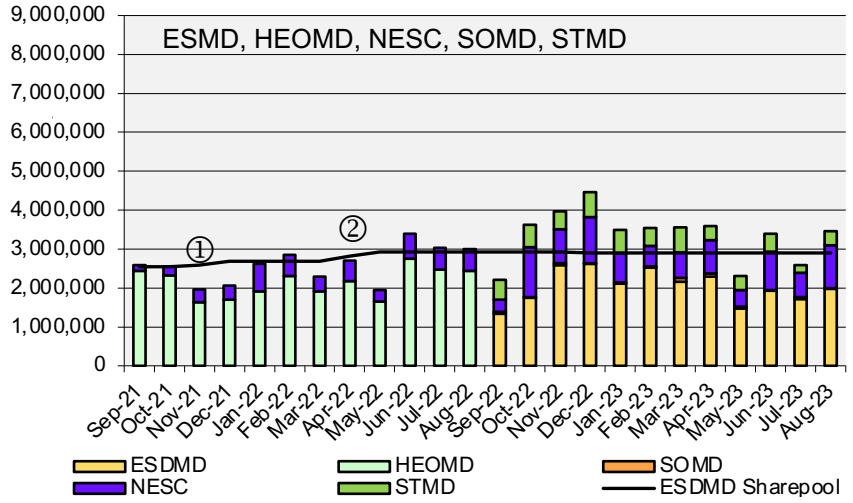
HECC Utilization Normalized to 30-Day Month



HECC Utilization Normalized to 30-Day Month



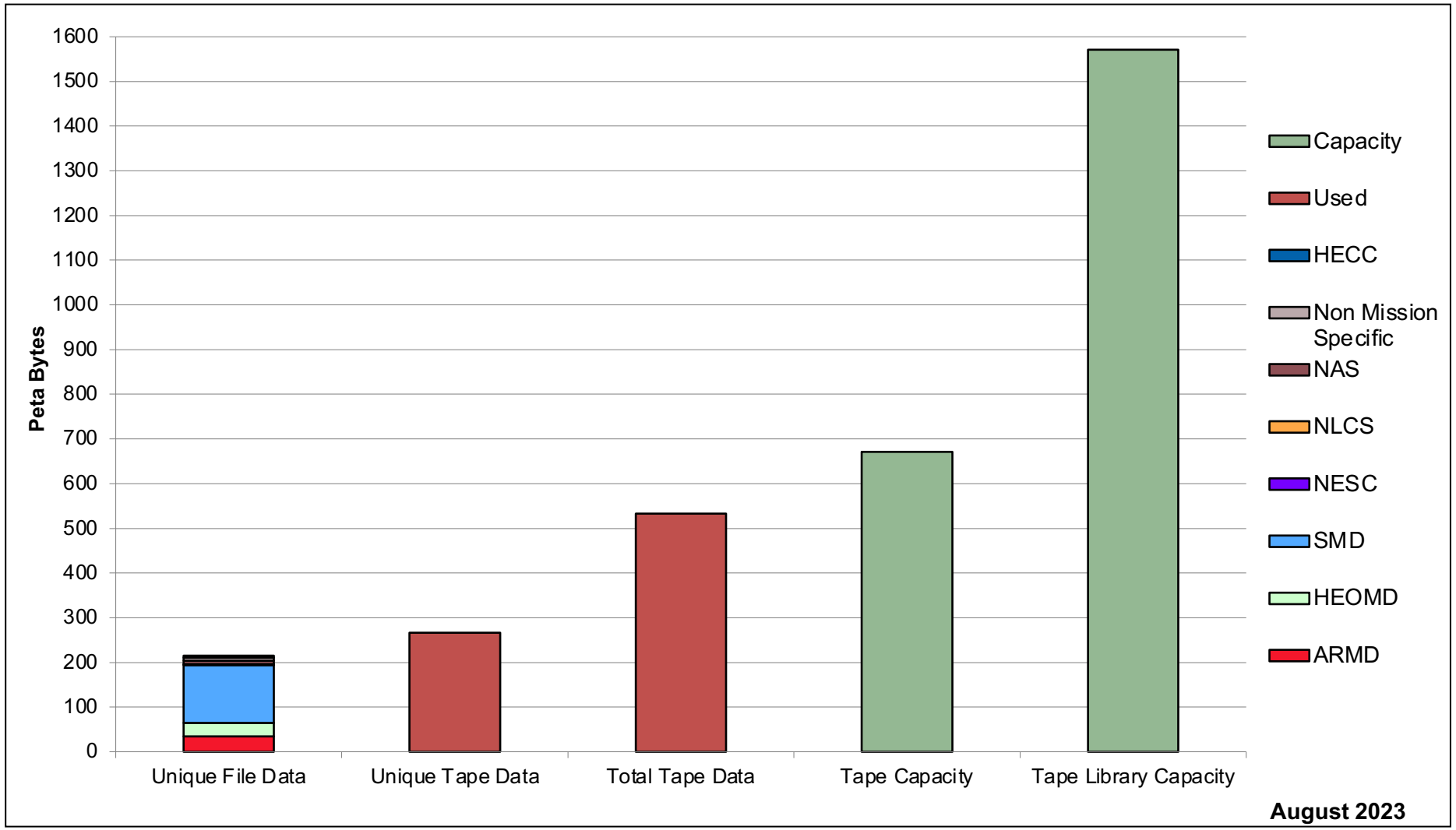




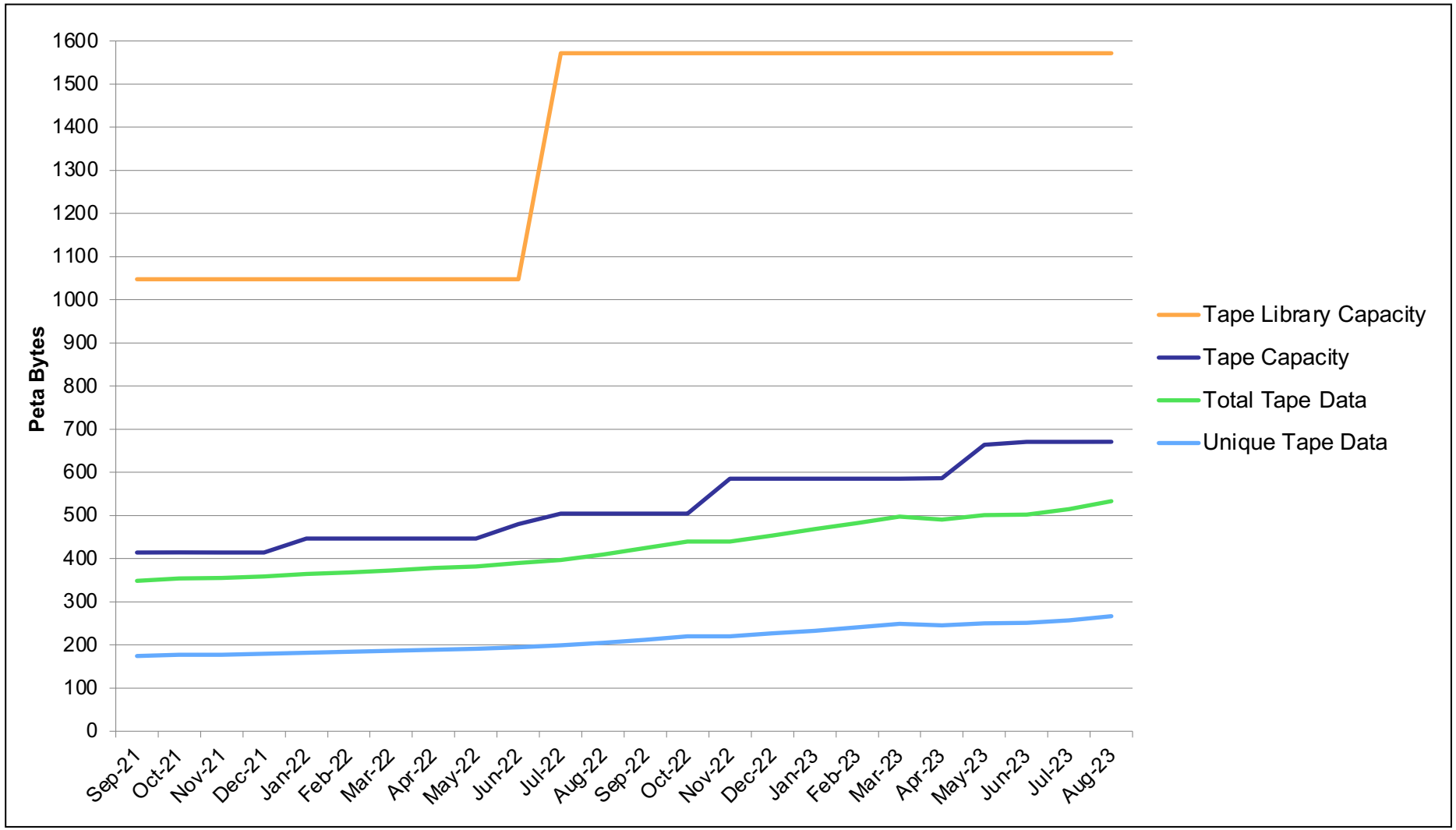
① 4 Rome Apollo Racks added to Aitken

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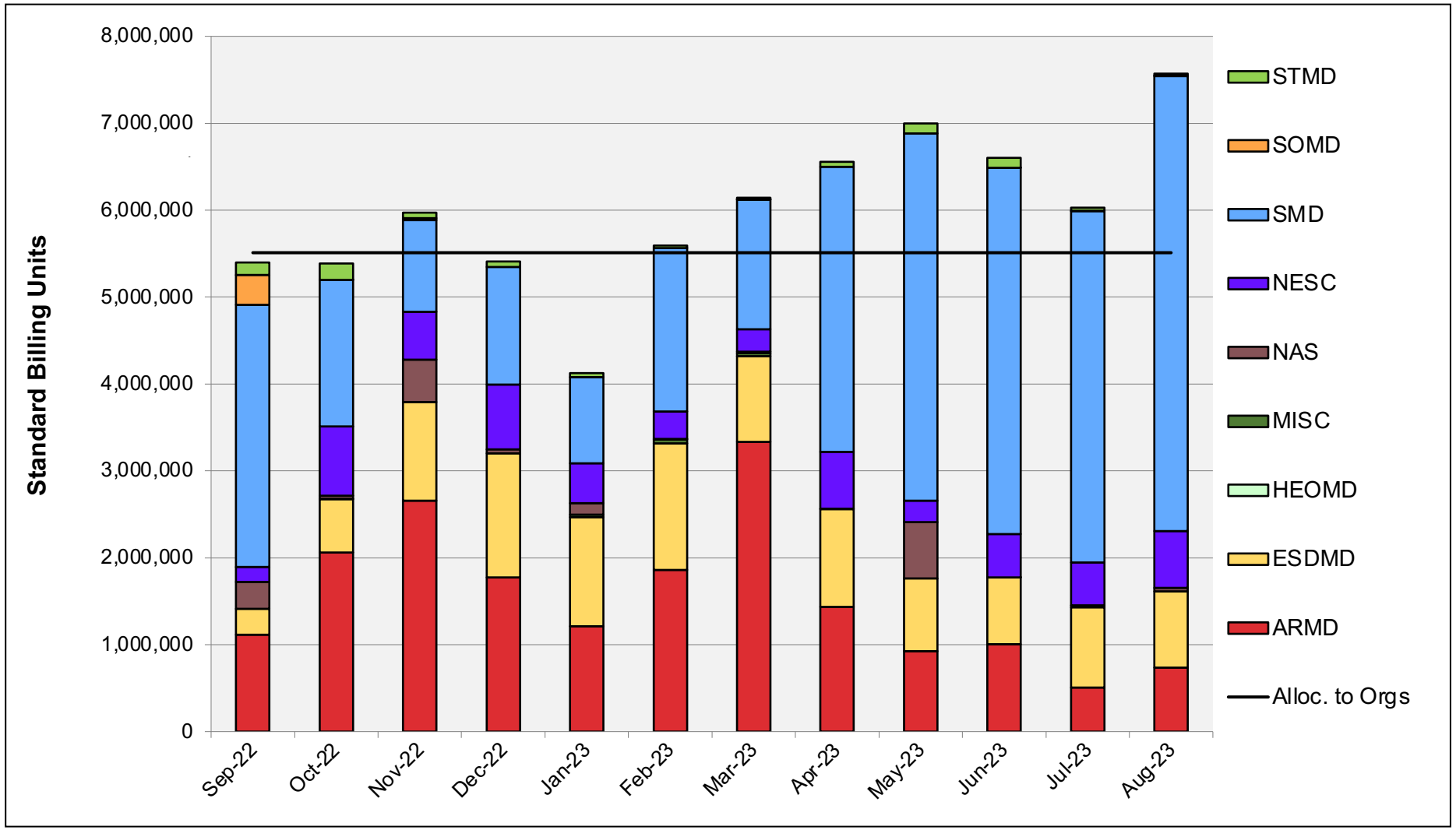
Tape Archive Status



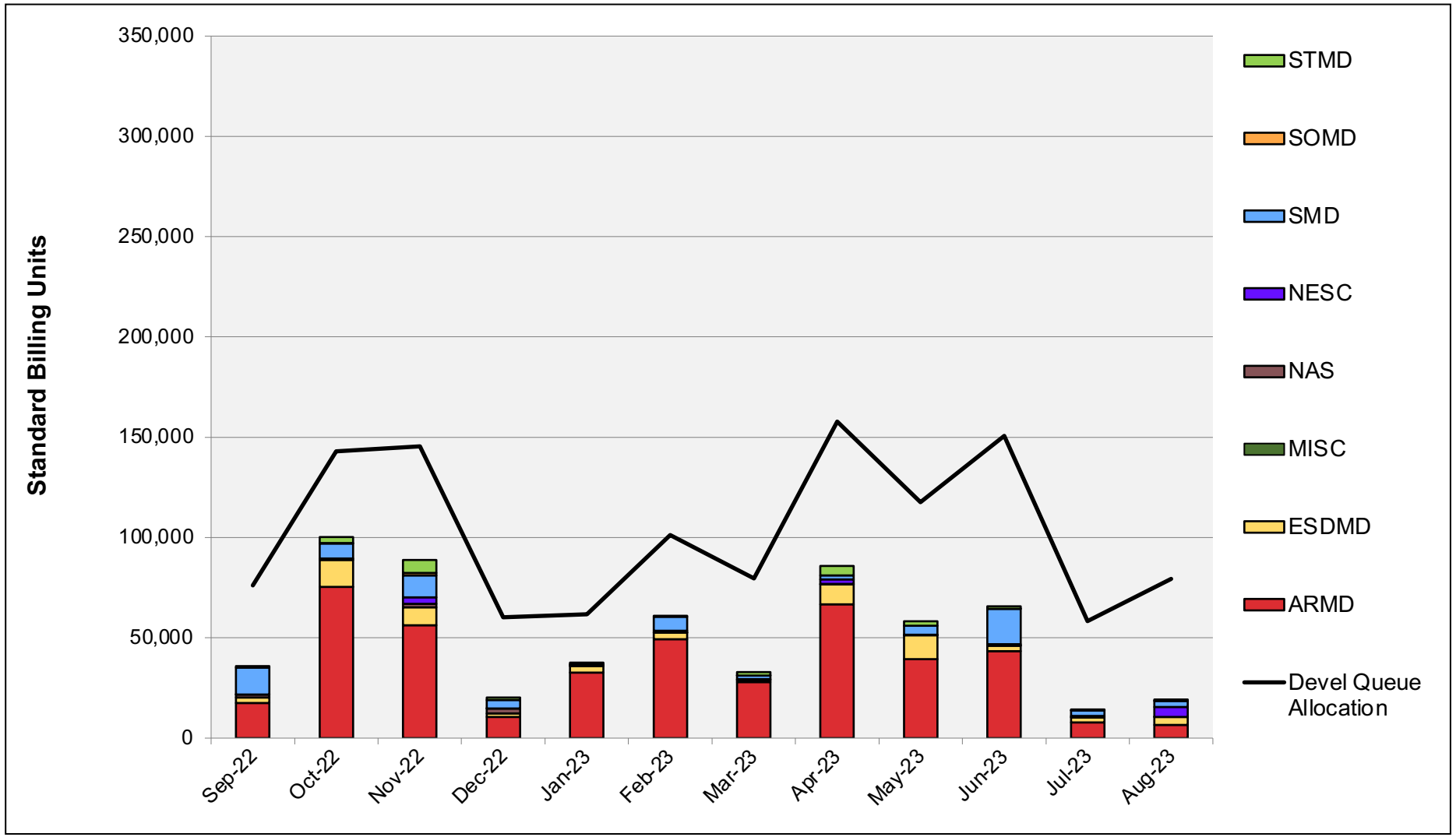
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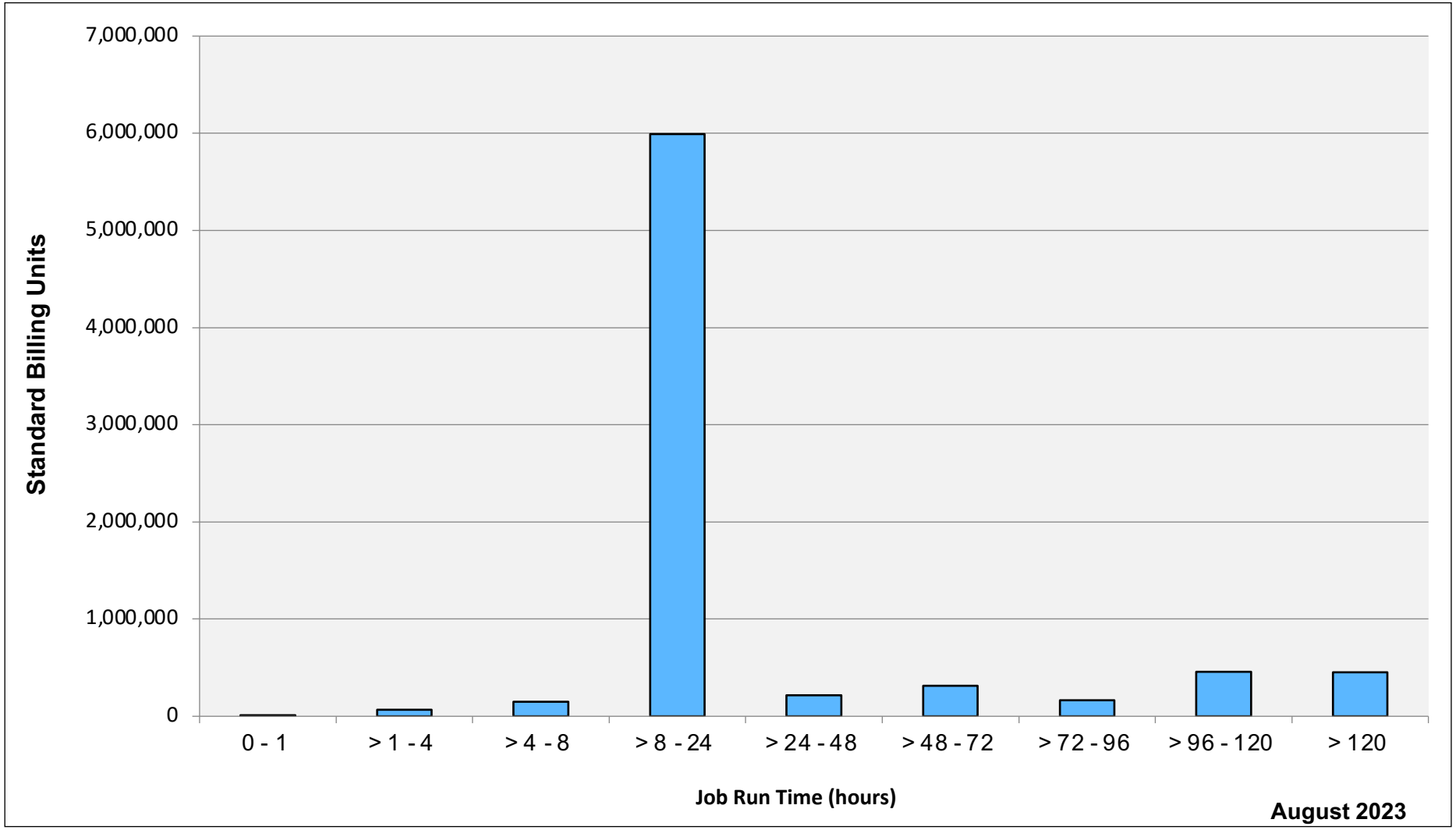
Aitken: SBUs Reported, Normalized to 30-Day Month



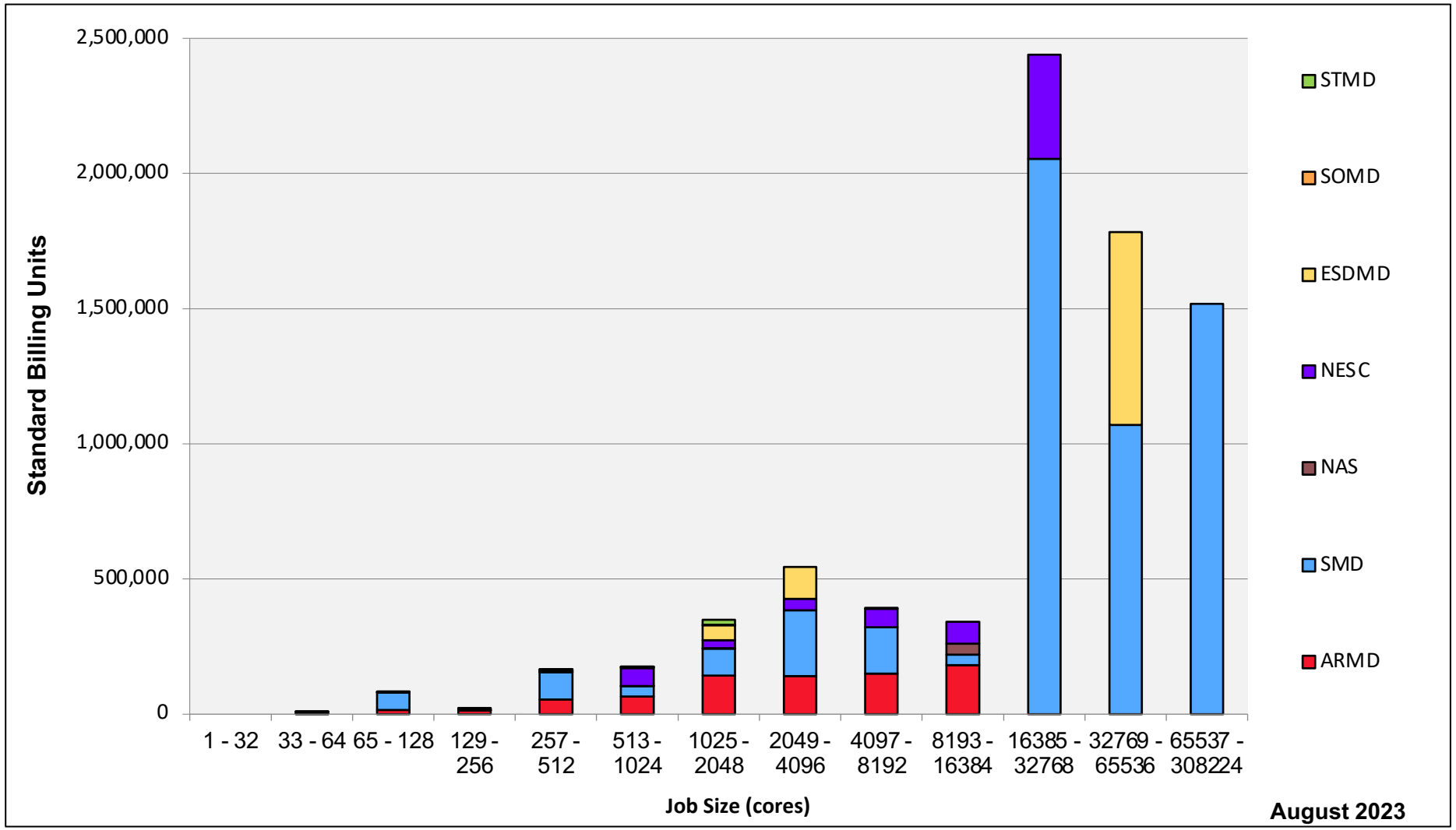
Aitken: Devel Queue Utilization



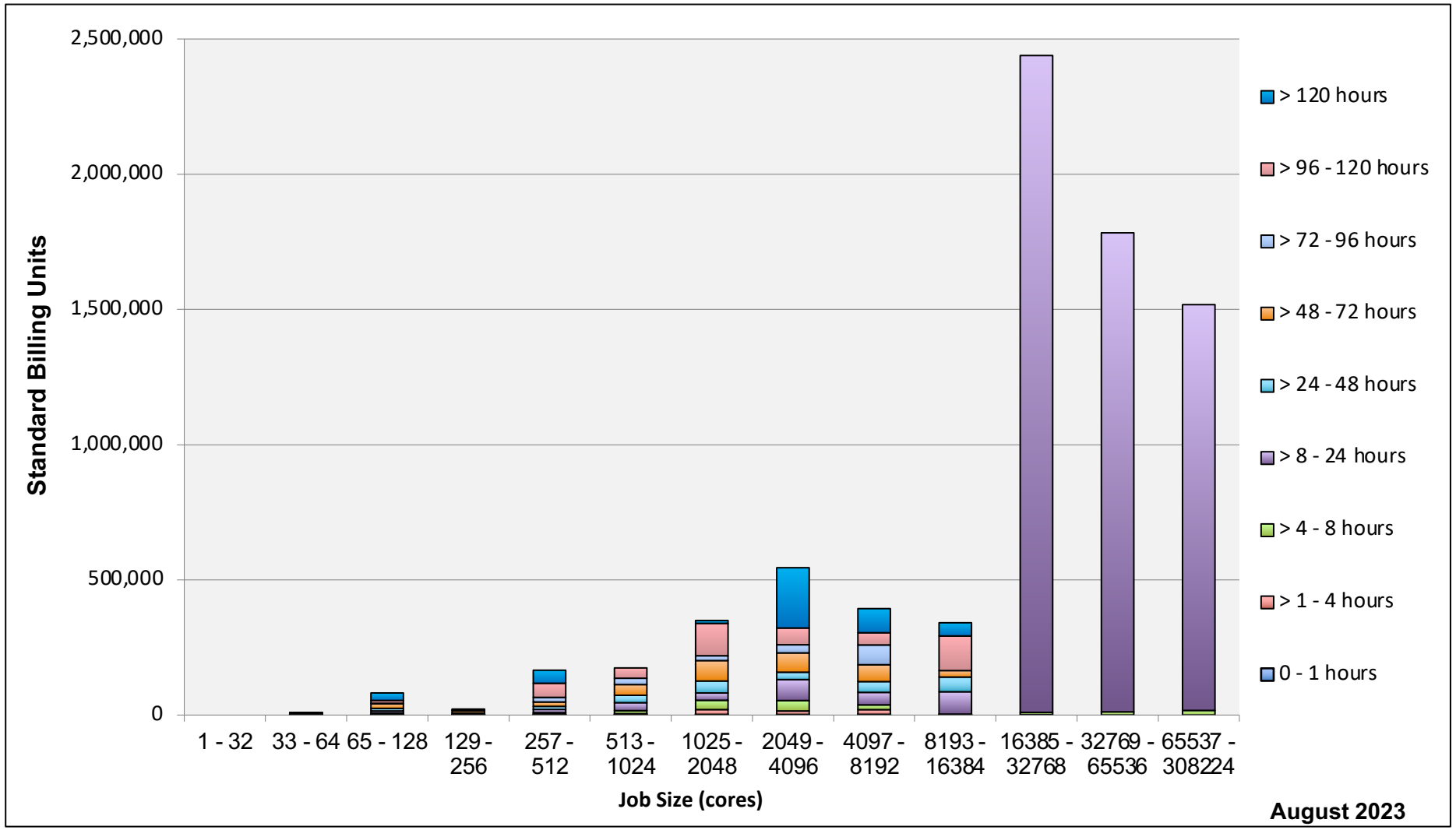
Aitken: Monthly Utilization by Job Length



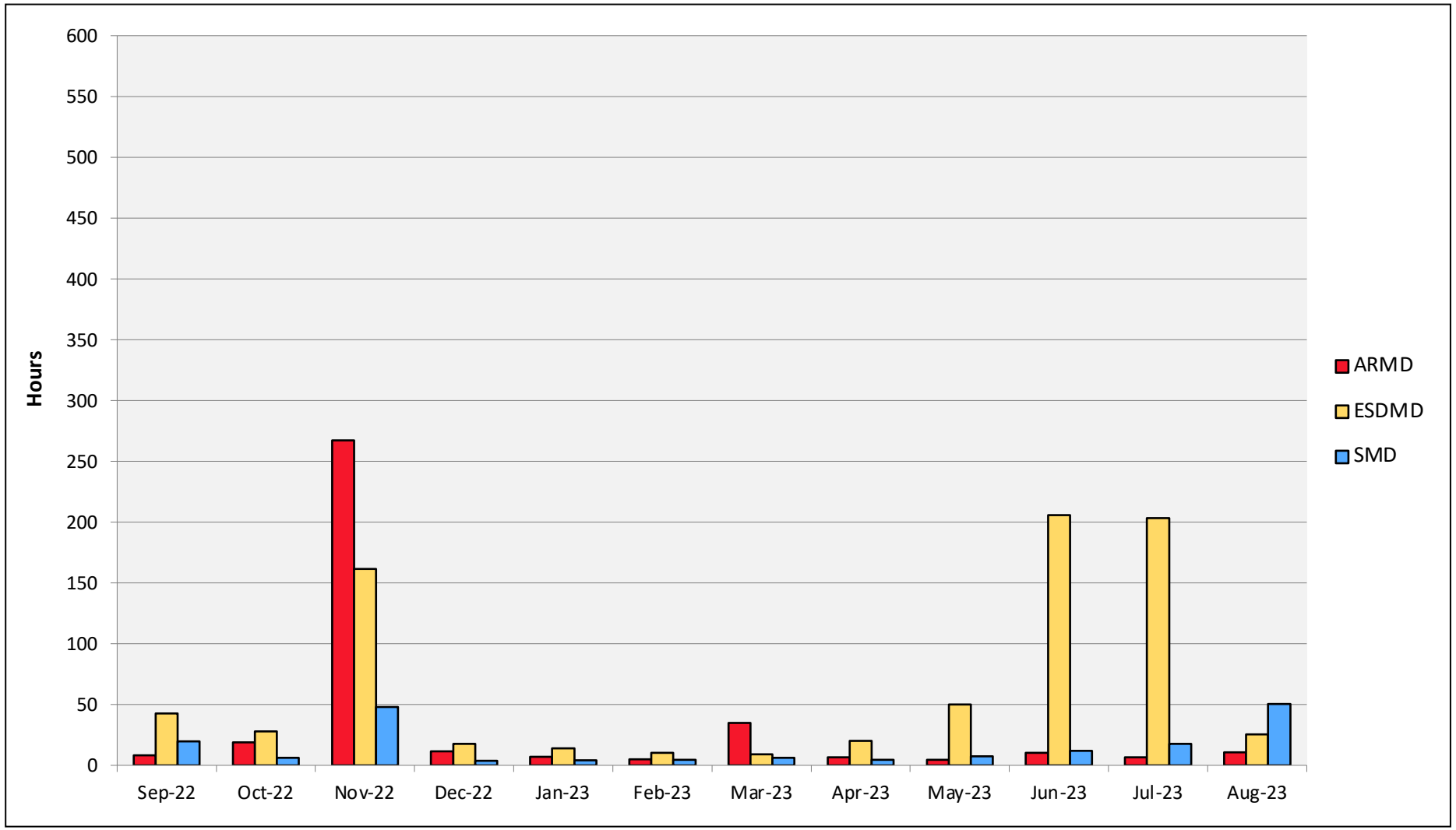
Aitken: Monthly Utilization by Job Size



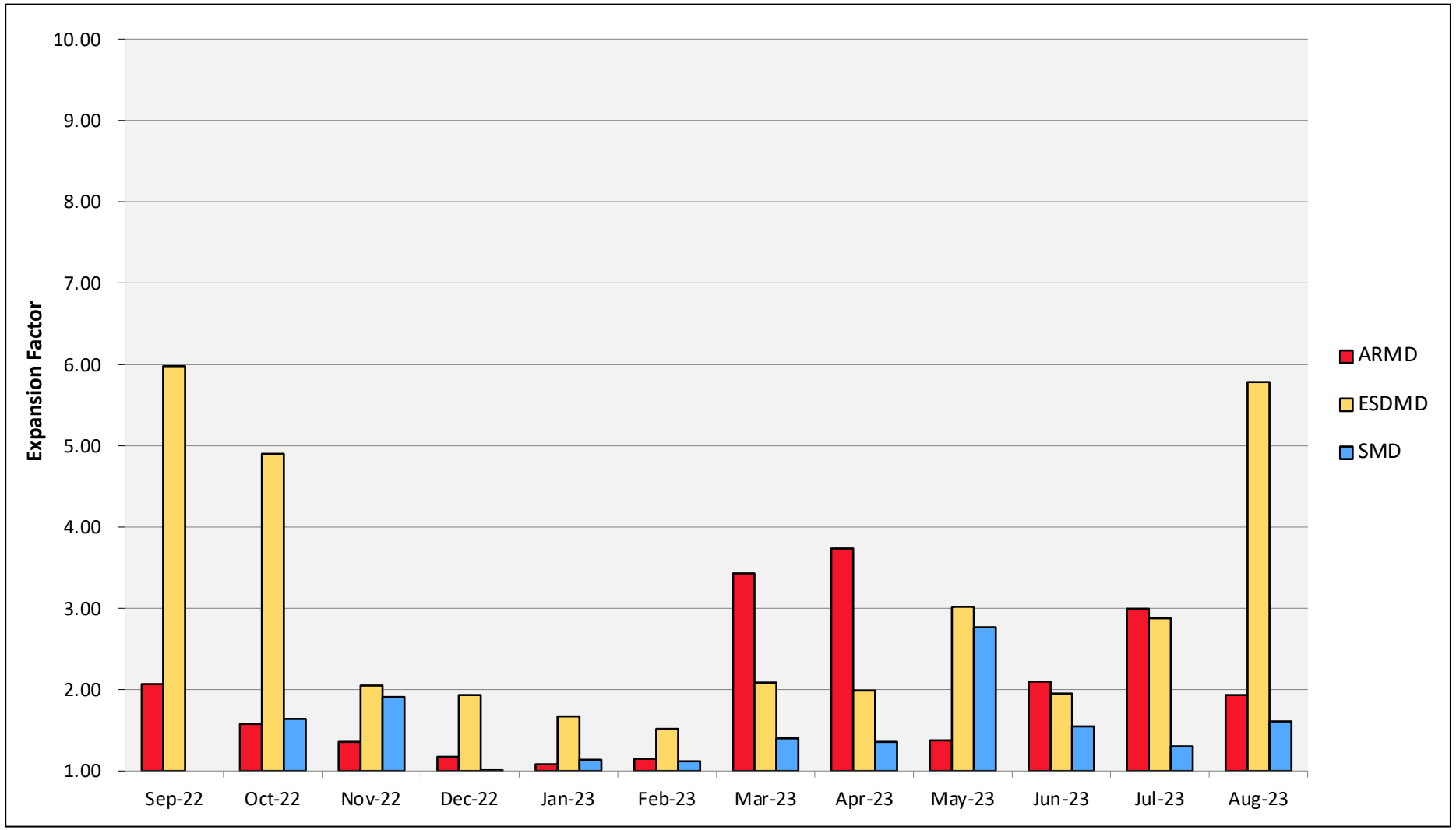
Aitken: Monthly Utilization by Size and Length



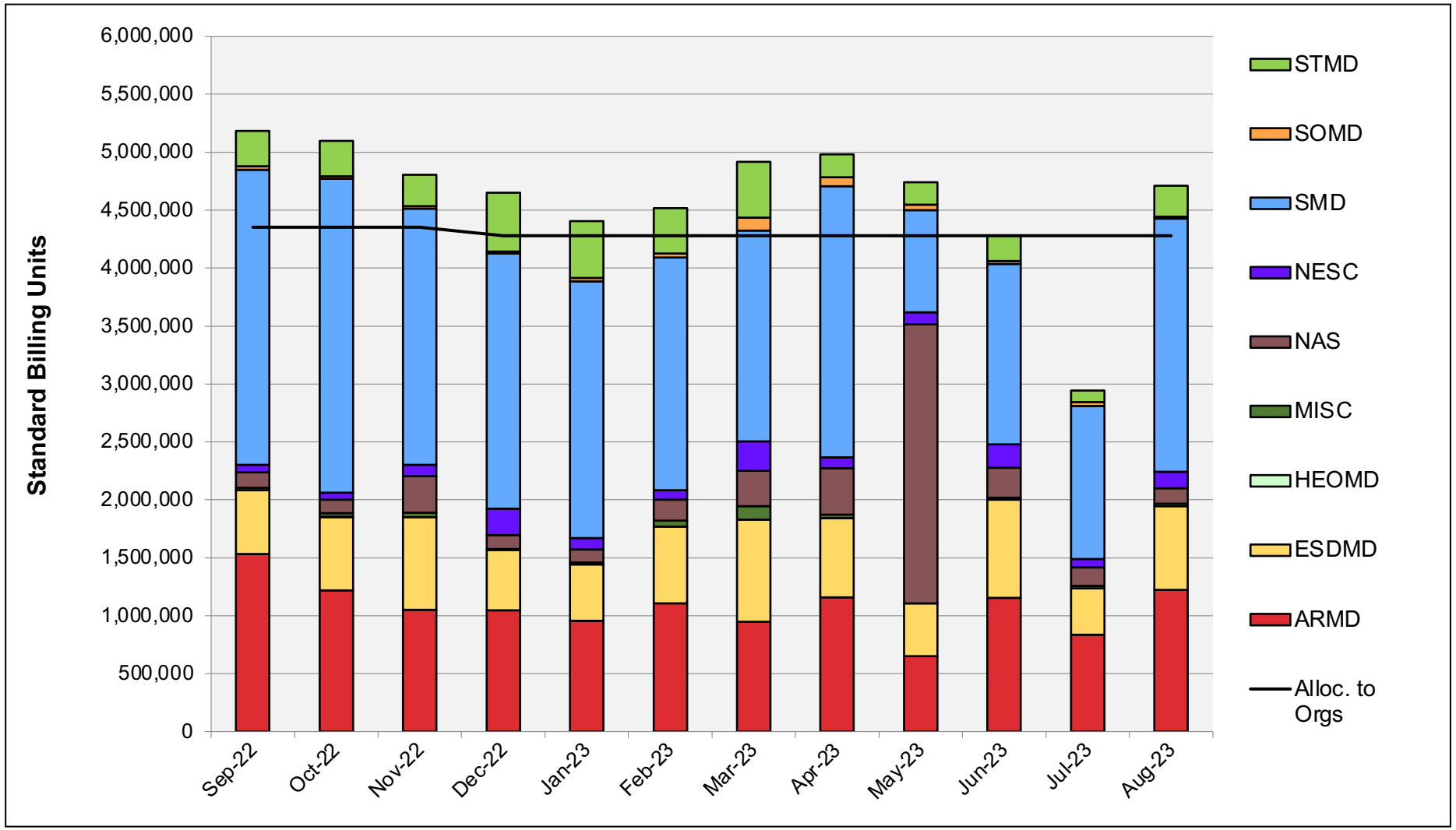
Aitken: Average Time to Clear All Jobs



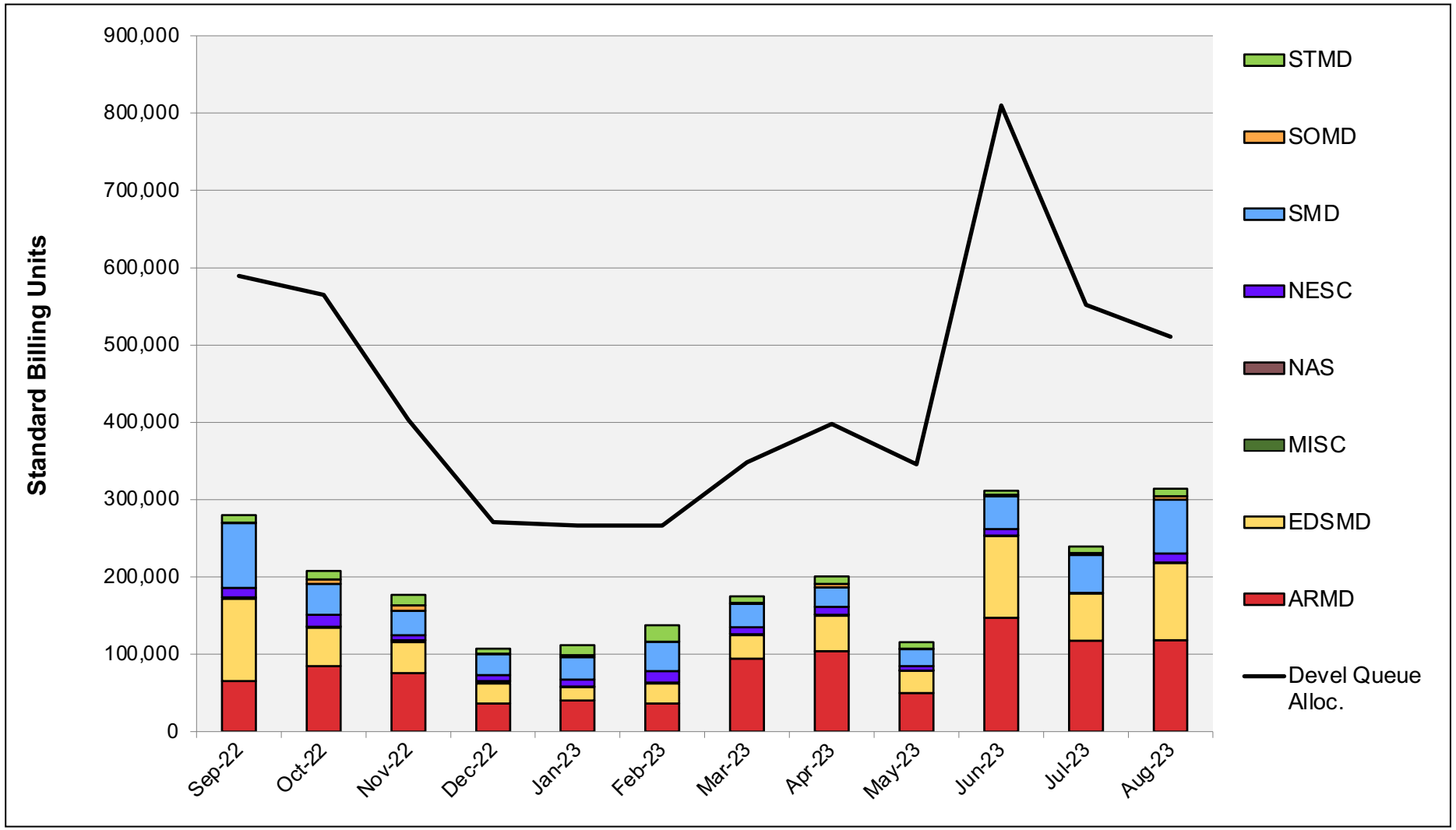
Aitken: Average Expansion Factor



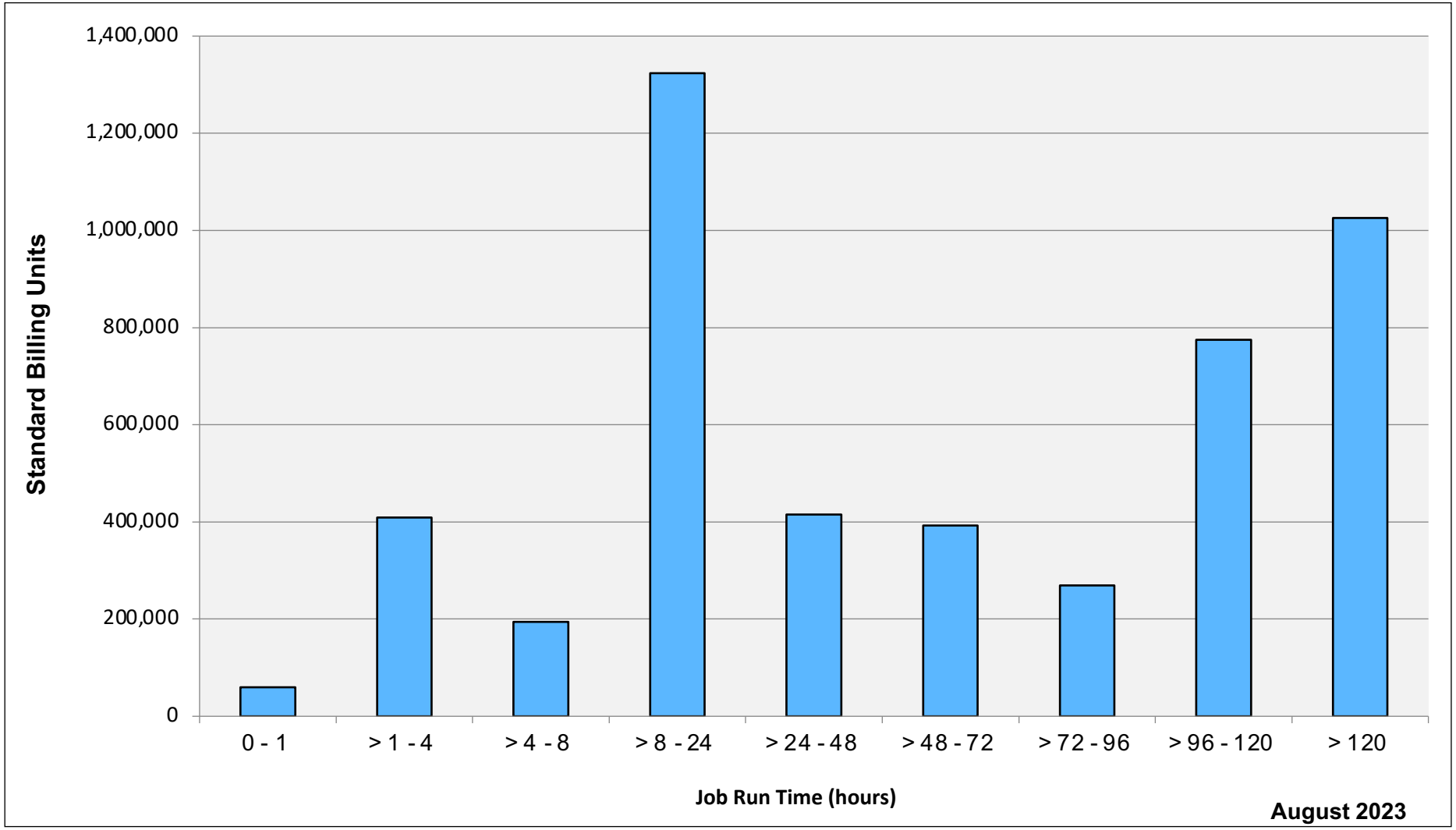
Pleiades: SBUs Reported, Normalized to 30-Day Month



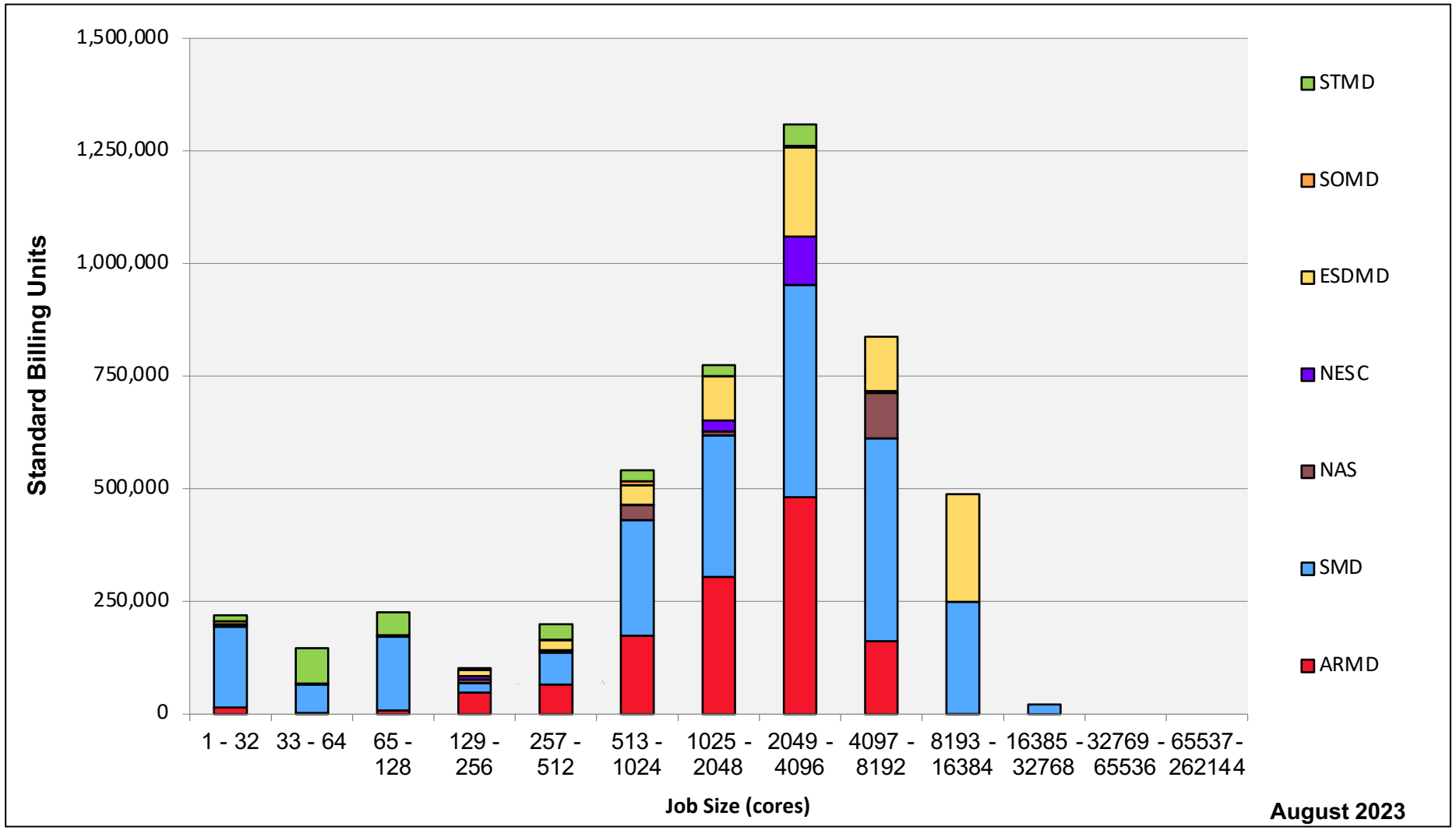
Pleiades: Devel Queue Utilization



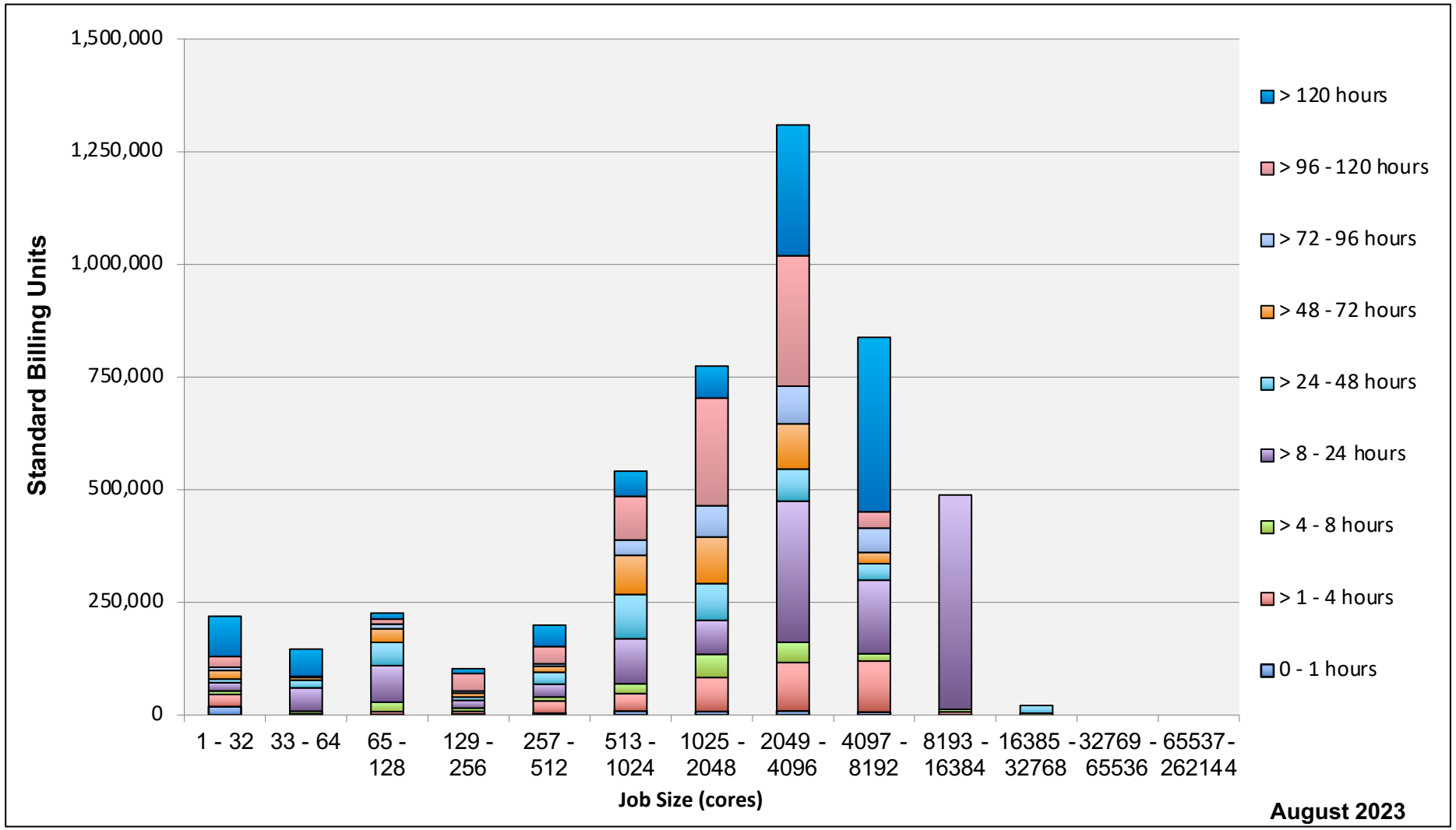
Pleiades: Monthly Utilization by Job Length



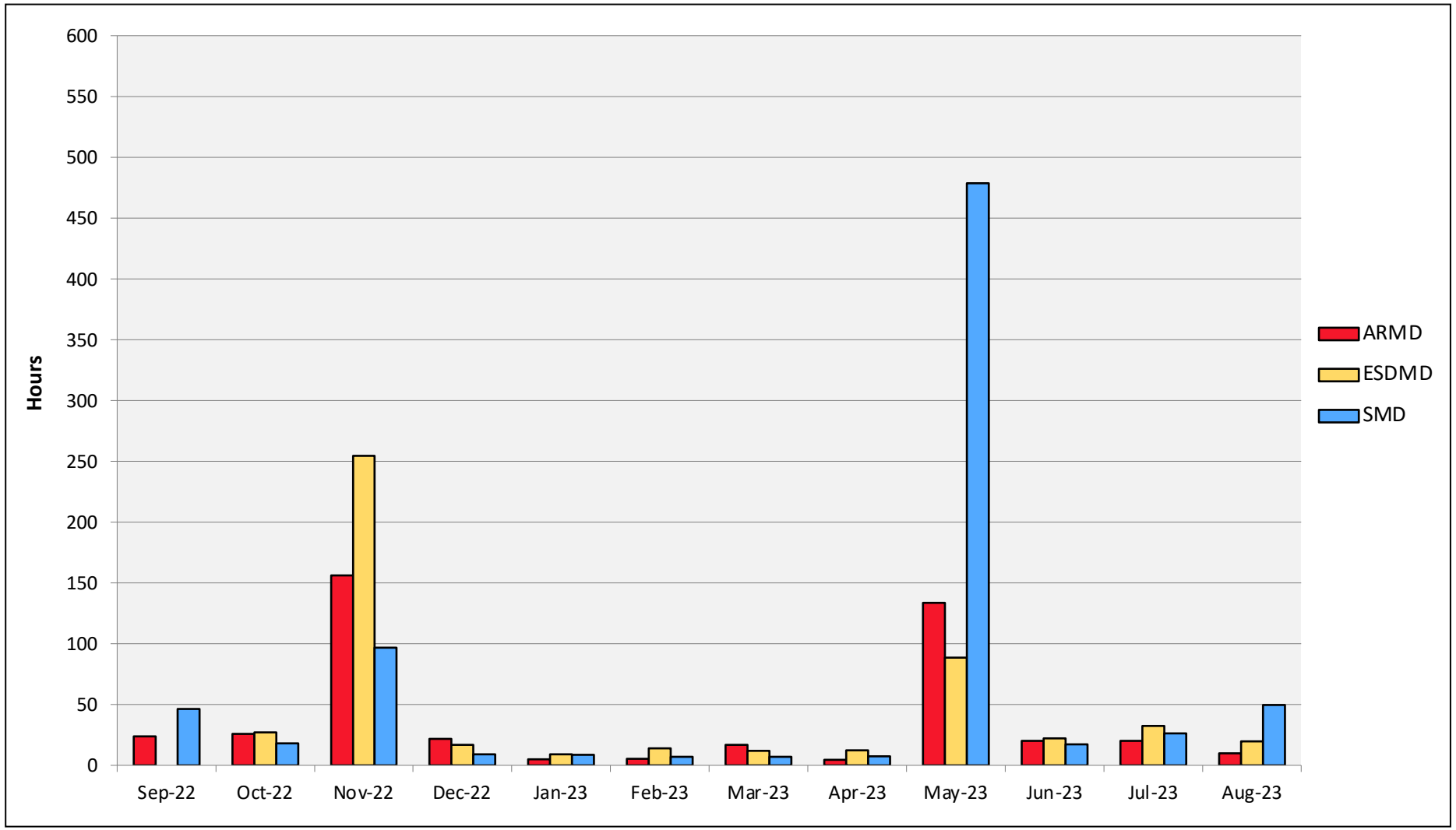
Pleiades: Monthly Utilization by Job Size



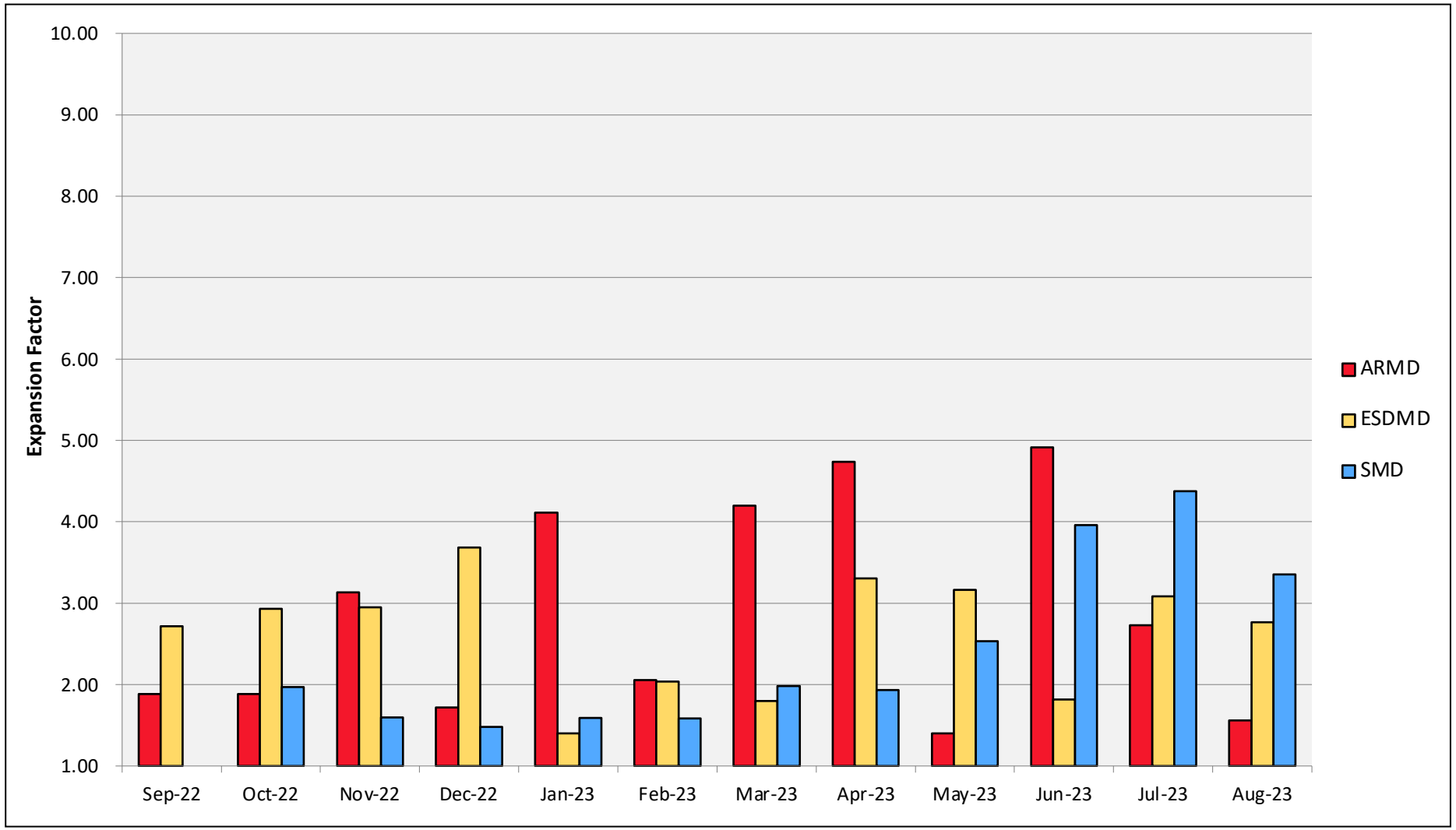
Pleiades: Monthly Utilization by Size and Length



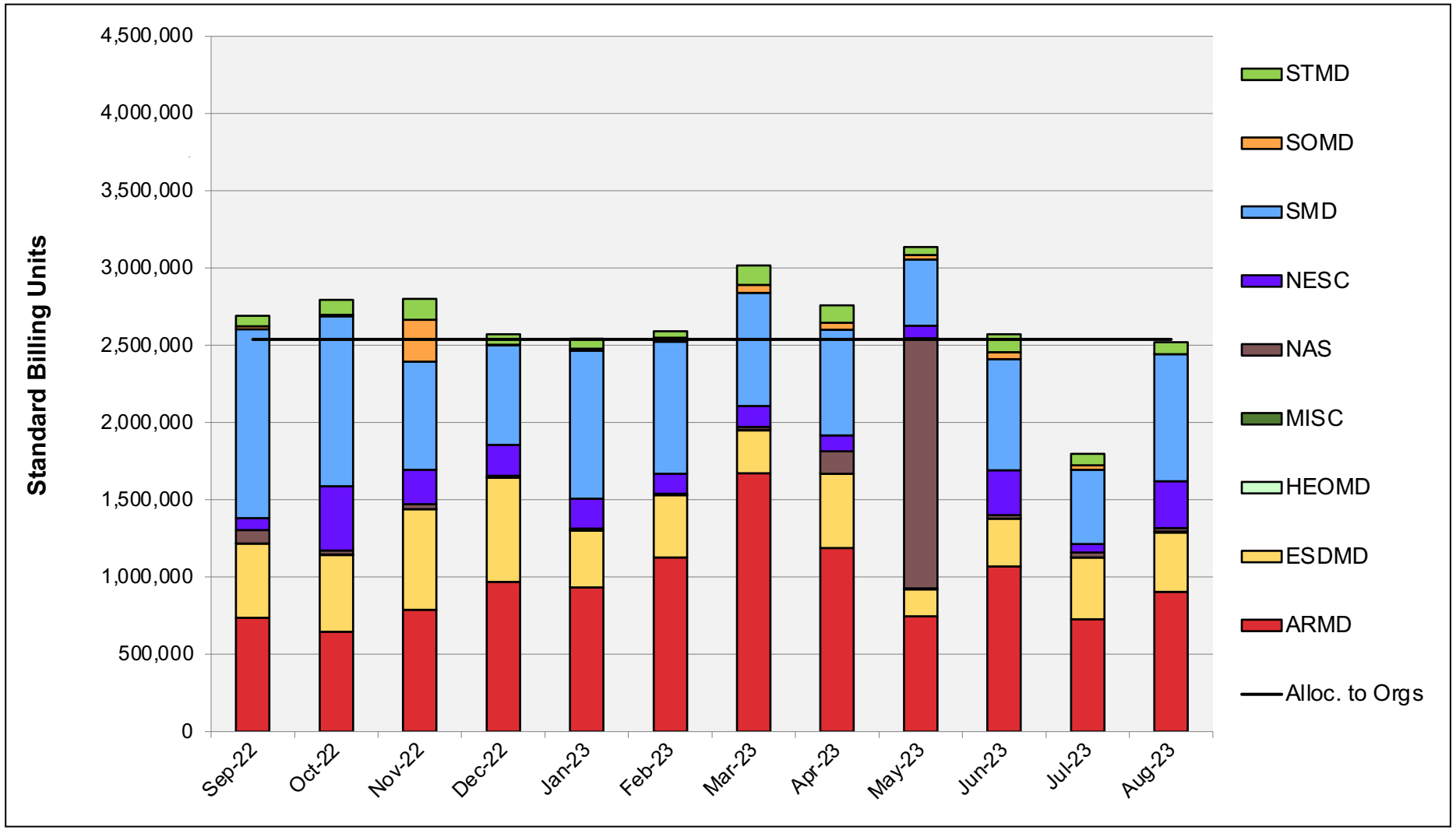
Pleiades: Average Time to Clear All Jobs



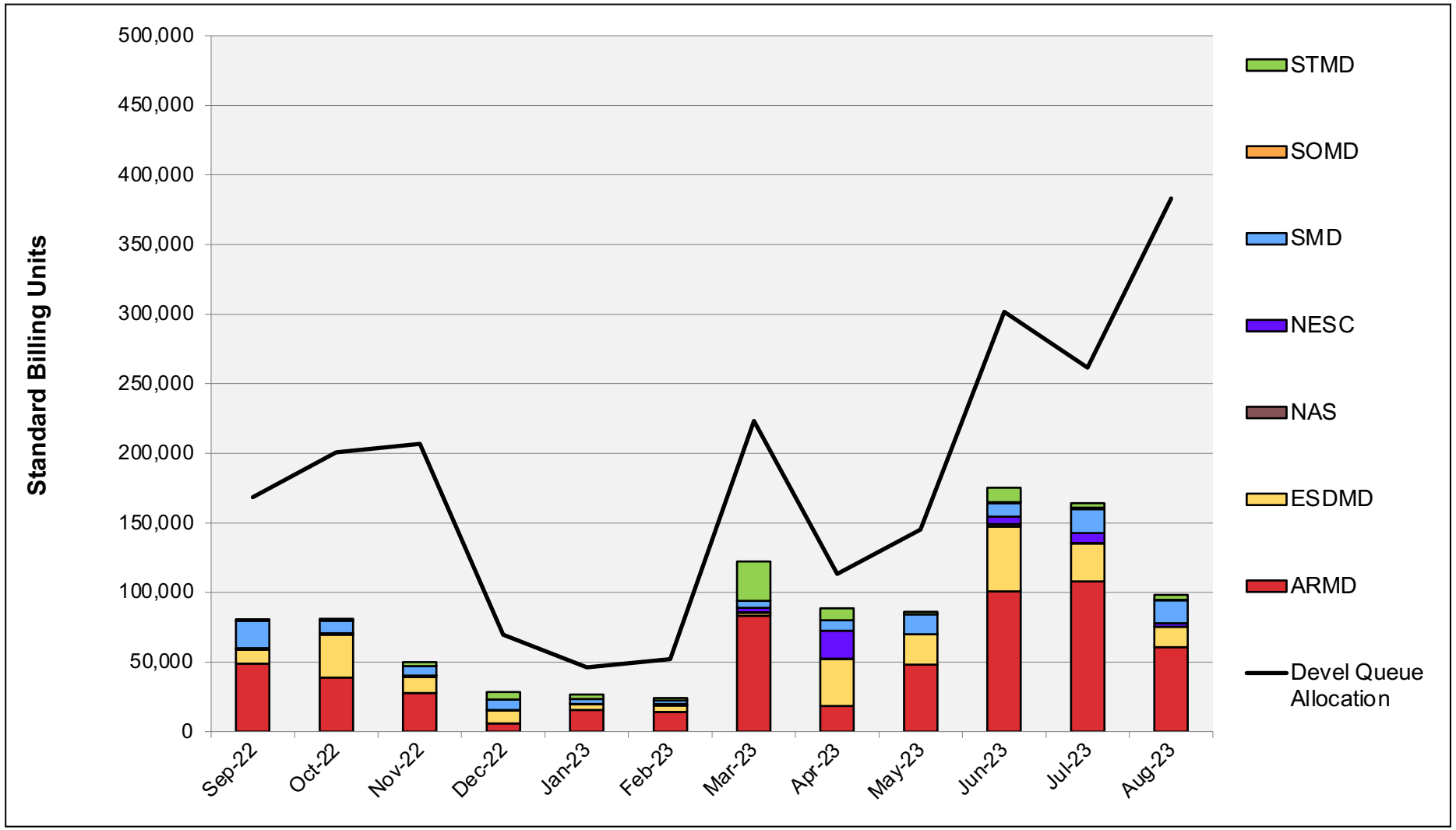
Pleiades: Average Expansion Factor



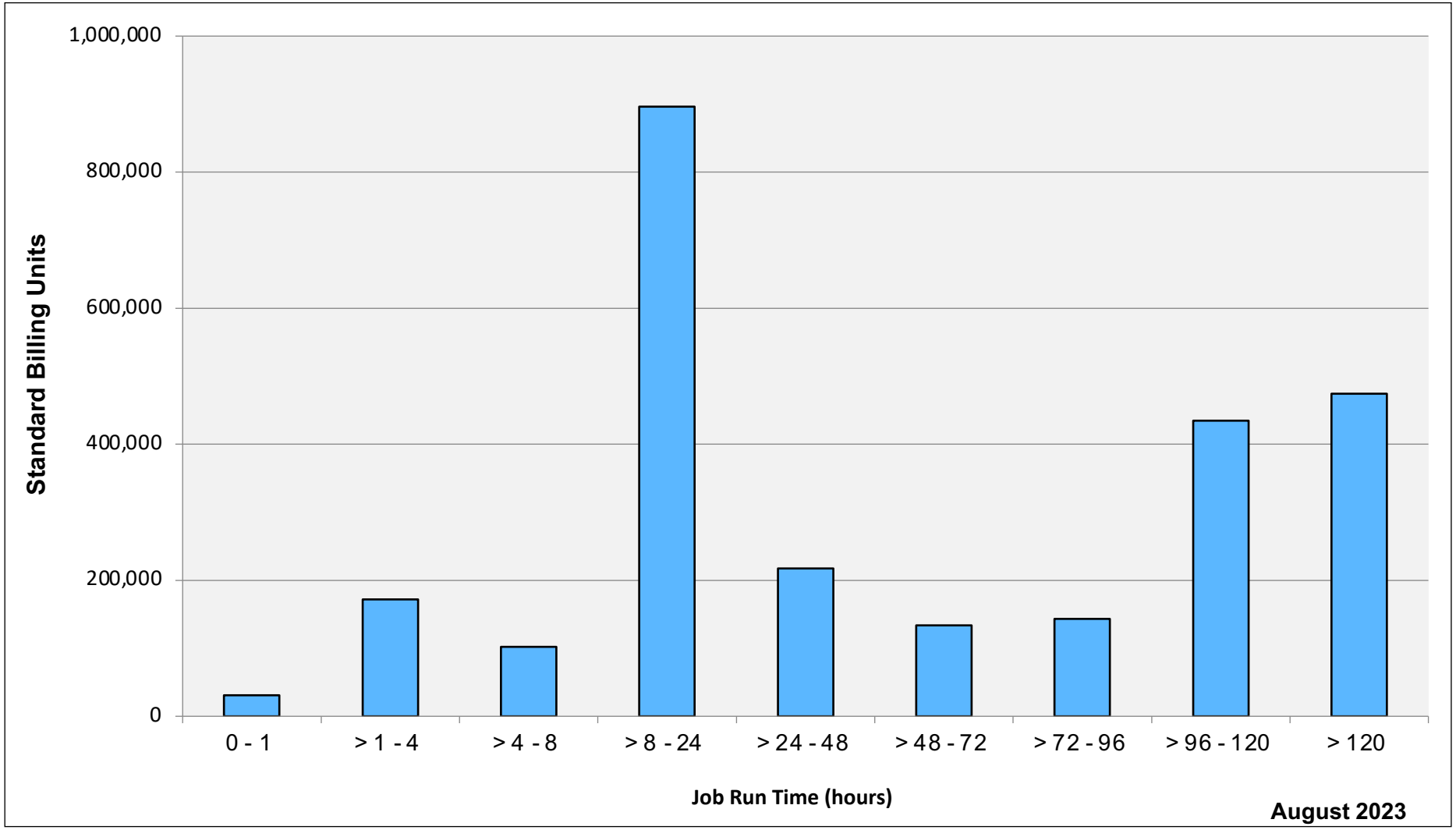
Electra: SBUs Reported, Normalized to 30-Day Month



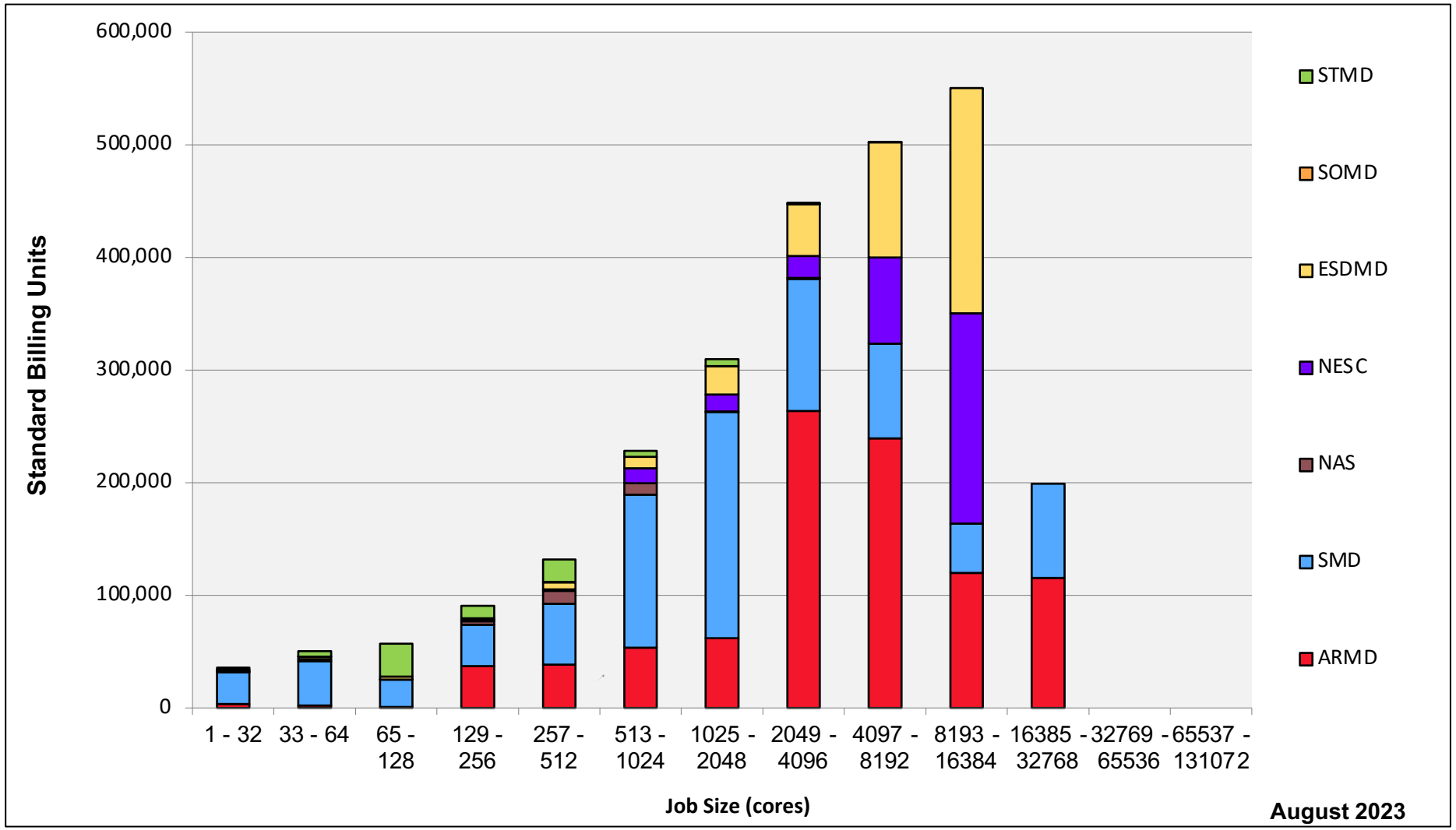
Electra: Devel Queue Utilization



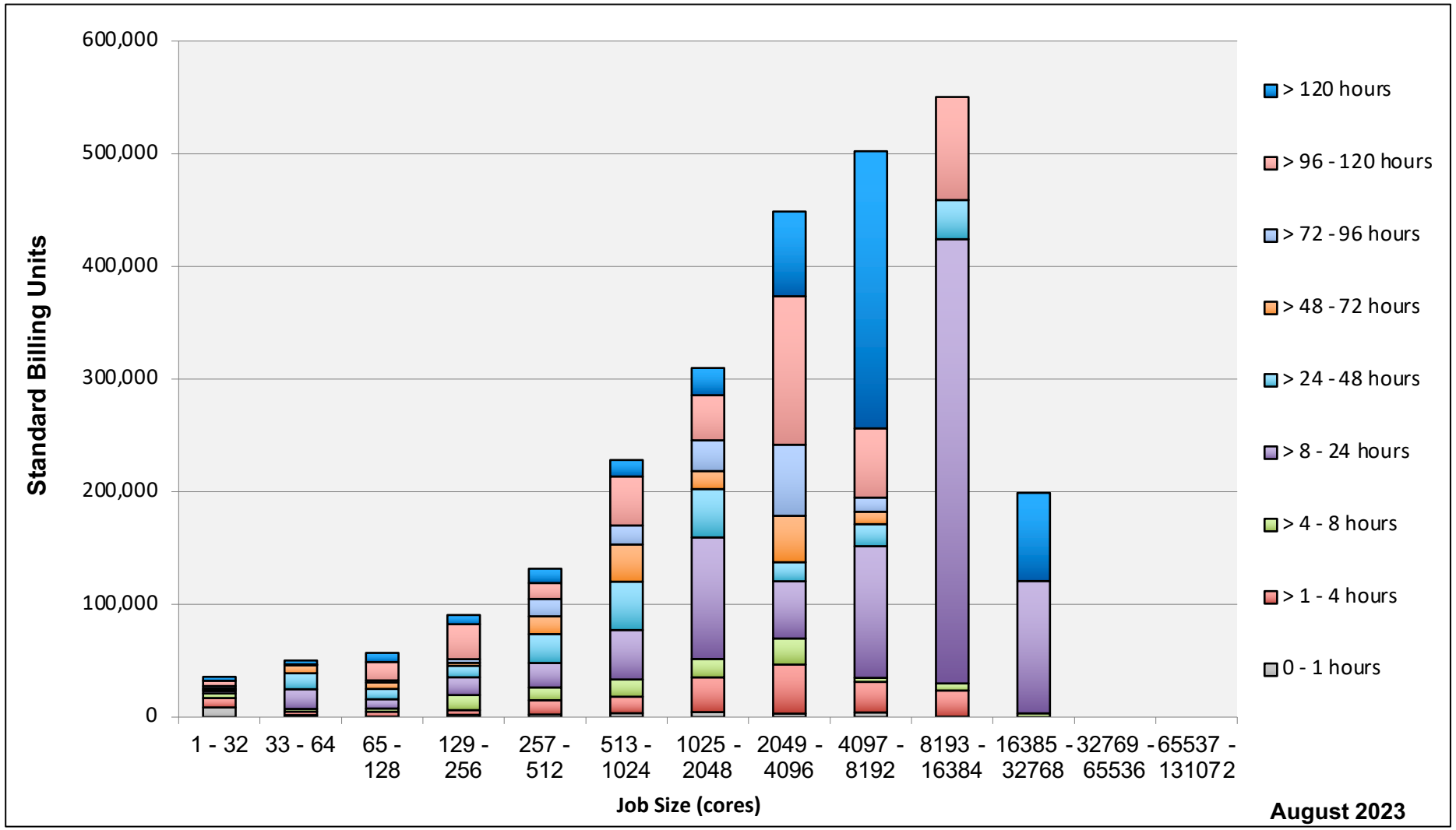
Electra: Monthly Utilization by Job Length



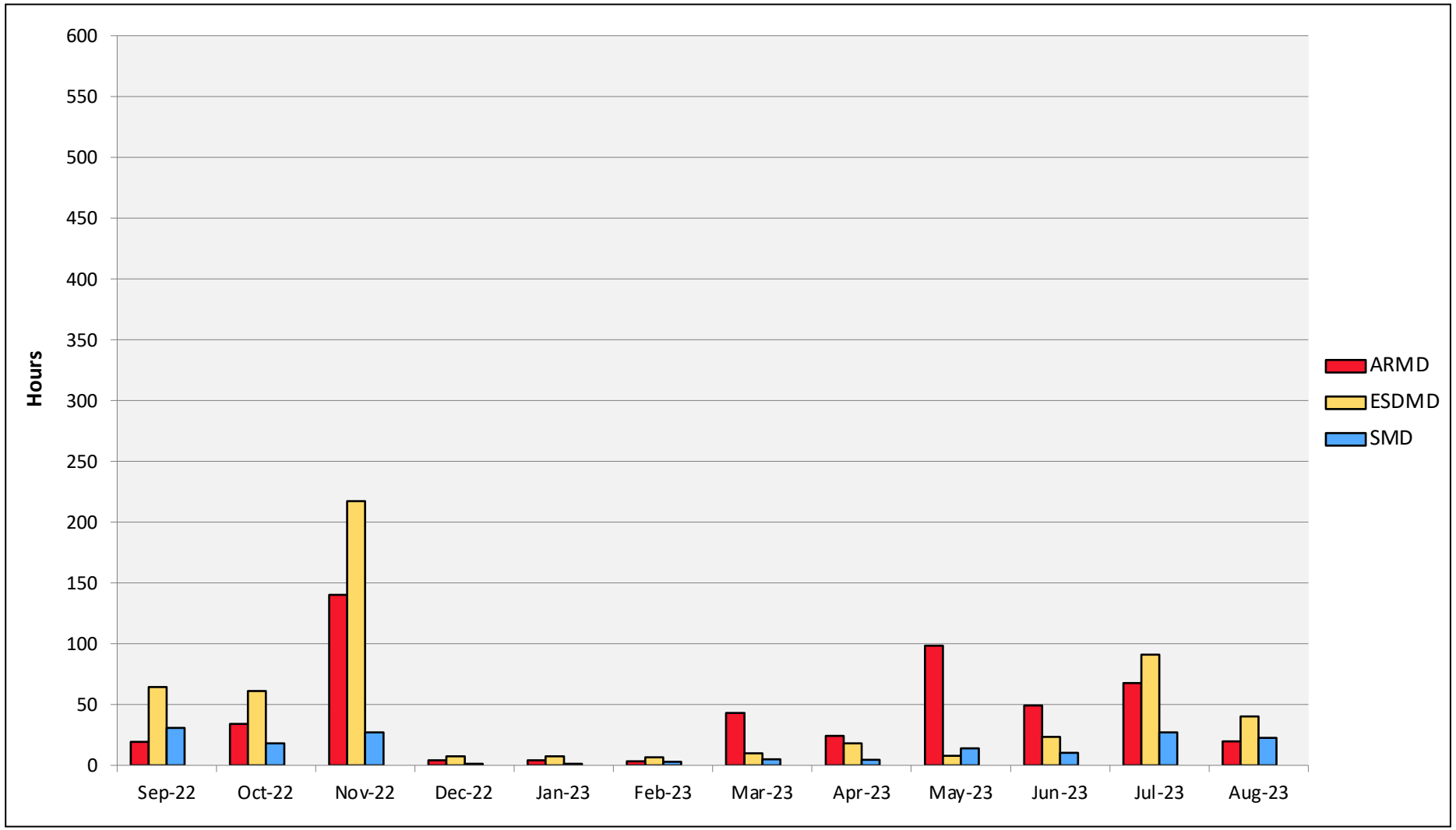
Electra: Monthly Utilization by Job Size



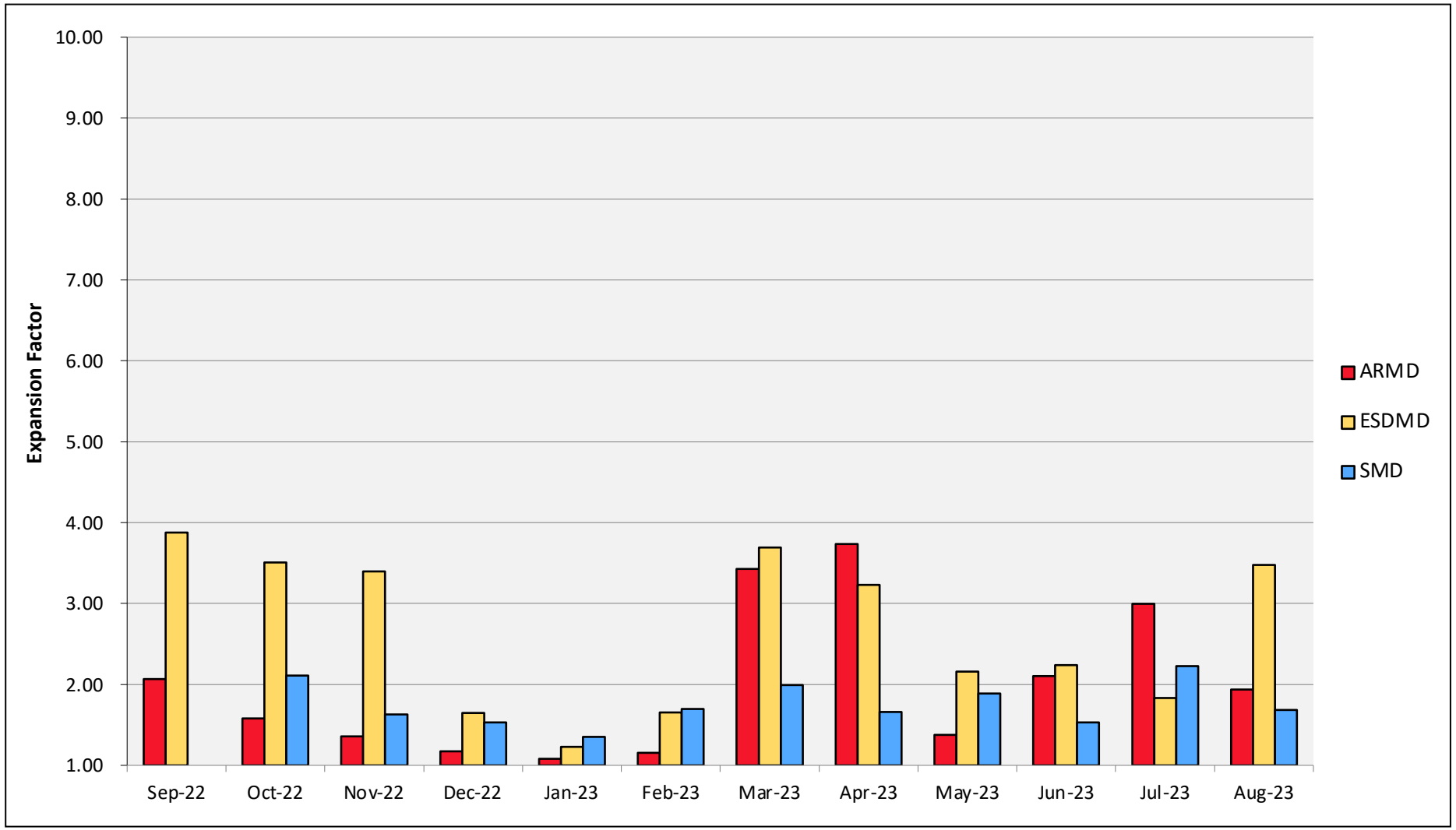
Electra: Monthly Utilization by Size and Length



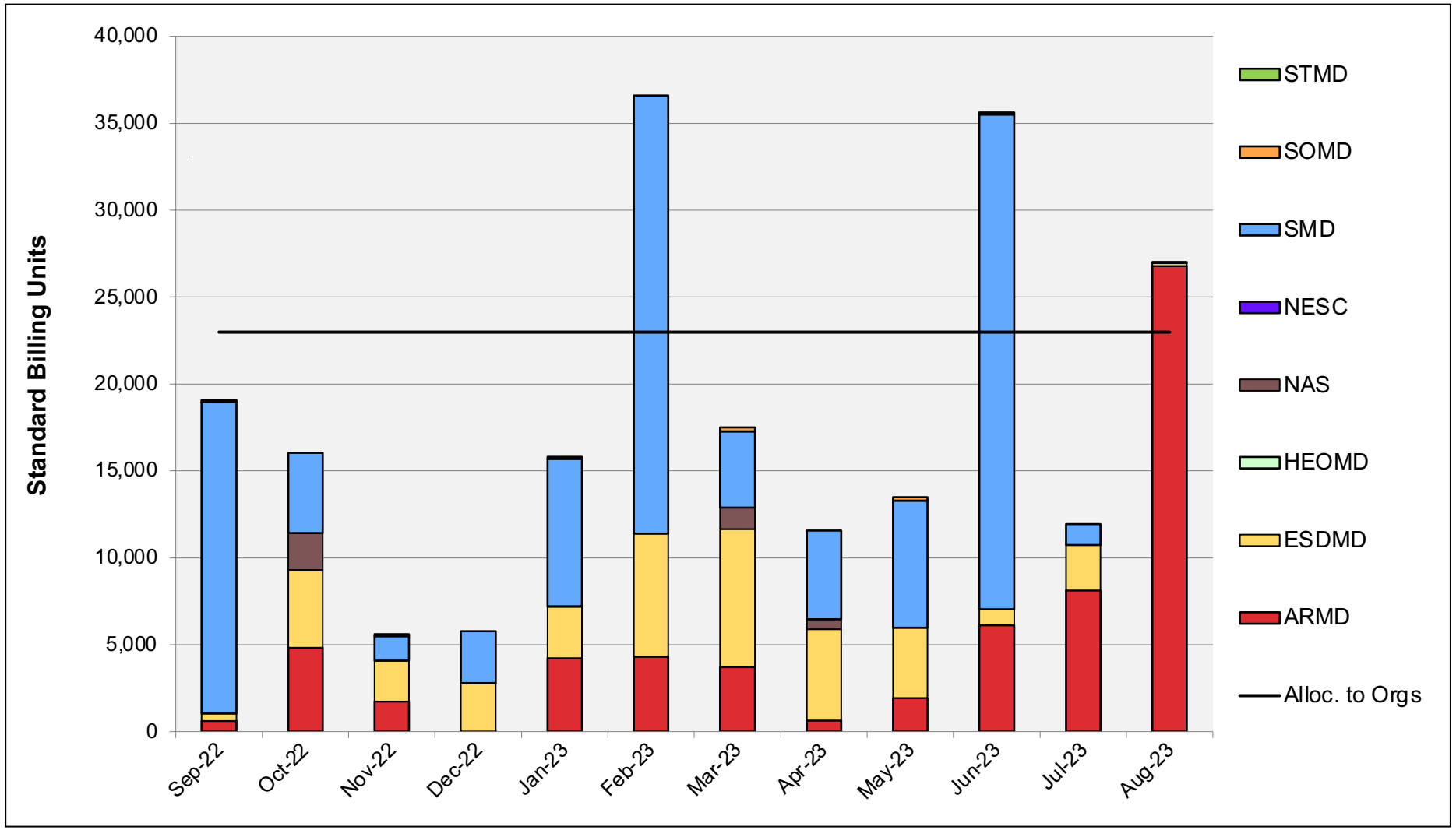
Electra: Average Time to Clear All Jobs



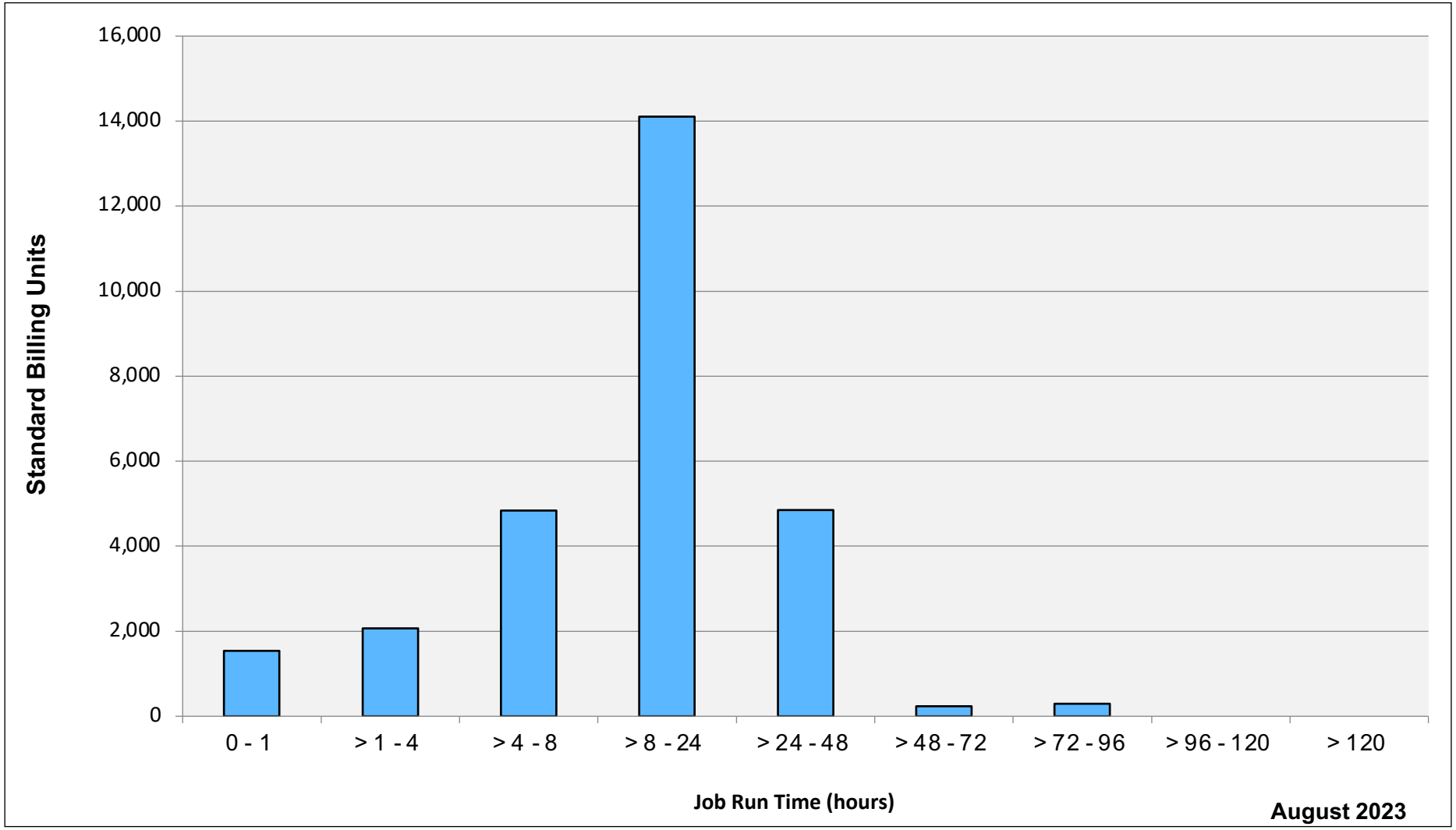
Electra: Average Expansion Factor



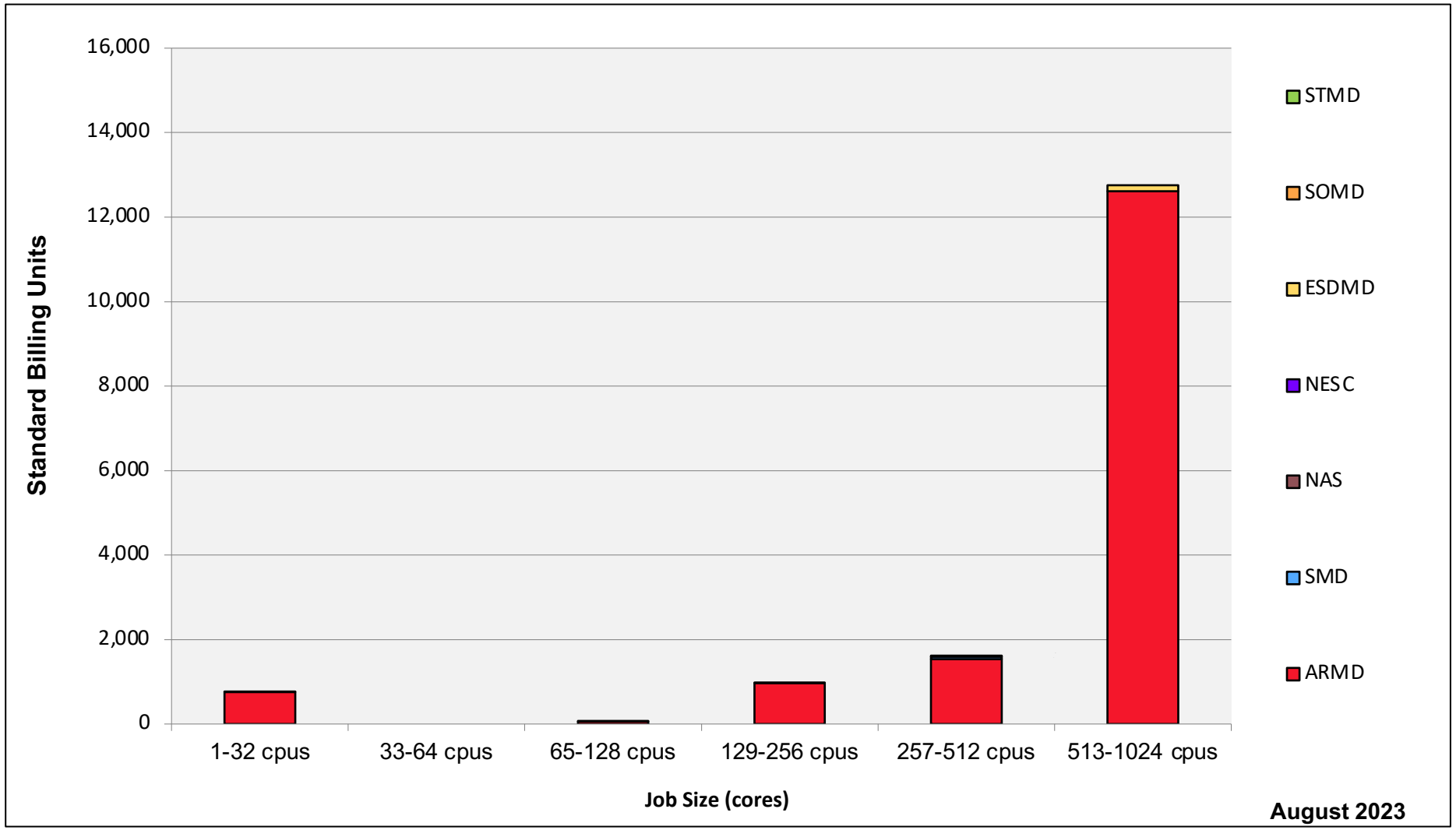
Endeavour: SBUs Reported, Normalized to 30-Day Month



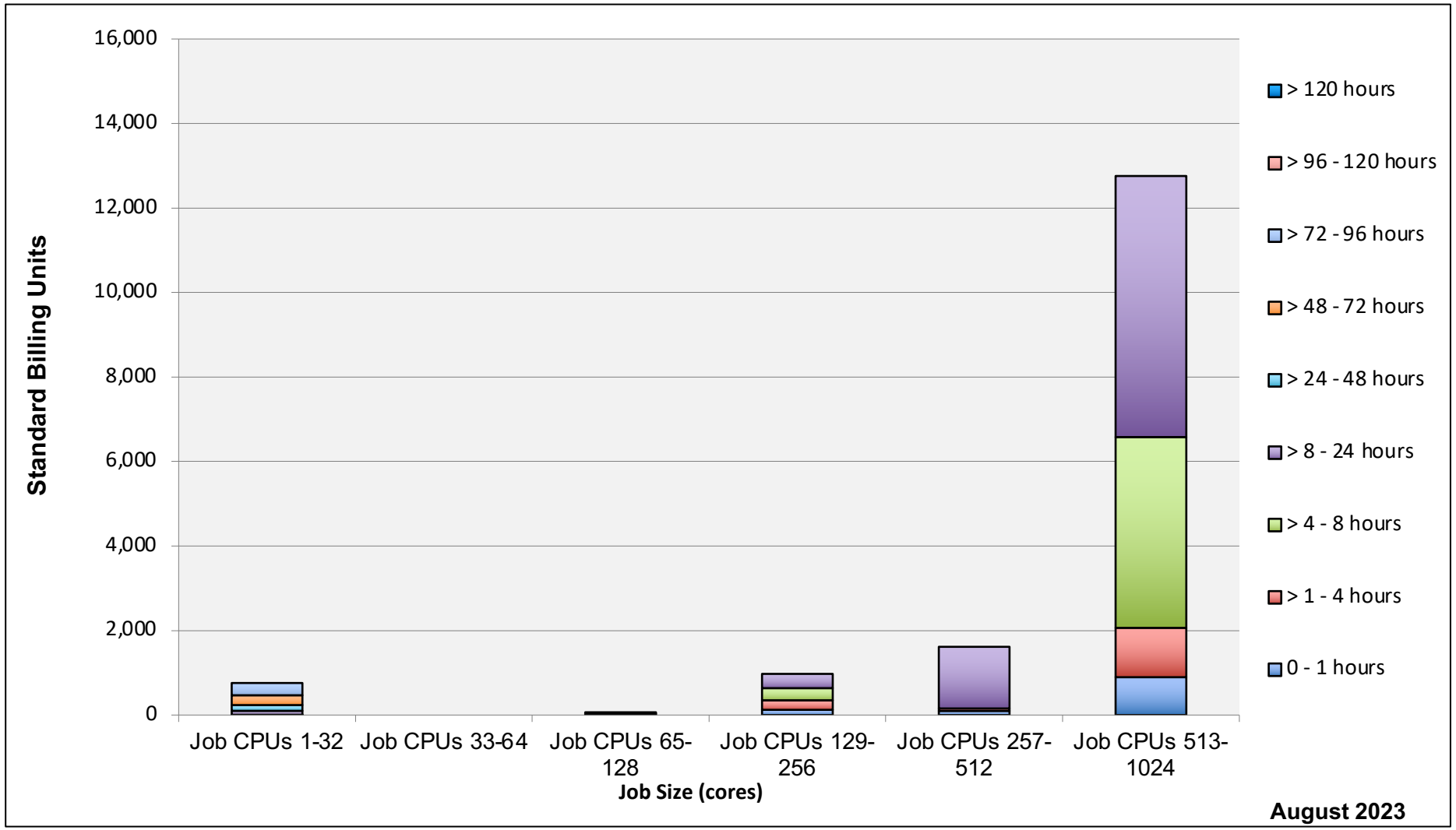
Endeavour: Monthly Utilization by Job Length



Endeavour: Monthly Utilization by Job Size



Endeavour: Monthly Utilization by Size and Length



Endeavour: Average Expansion Factor

