

National Aeronautics and Space Administration

HIGH-END COMPUTING CAPABILITY PORTFOLIO

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HECC Teams Complete Successful RHEL 8 Transition

- To ensure continued compliance with NASA cybersecurity requirements, the HECC RHEL 8 project team worked over 16 months to complete a complex migration of ~400 Linux systems to the Red Hat Enterprise Linux 8 (RHEL 8) operating system.
- The upgrade comprised multiple steps to transition each system to RHEL8: applying required agency security configurations; installing system-specific applications; and fully testing functionality, performance, and security.
- The team also completed two related projects, Hyperconverged Infrastructure (HCI) and Ansible configuration management, to significantly update NAS server and workstation infrastructure.
  - HCI works seamlessly and offers robust management tools, making it ideal for replacing many aging HECC physical servers with more powerful virtual machines at much less cost and in much less time.
  - The industry-standard Ansible tool enables scalable management of a large number of systems, providing improved flexibility and ease of use over the previous configuration management tool.
- The Tools, Networks, and Engineering Servers and Services groups worked as one team to meet numerous technical challenges and complete the work a month ahead of schedule.

IMPACT: The successful migration to RHEL 8 is the culmination of an extensive endeavor that resulted in a modern Linux infrastructure that provides significant improvement of HECC security standards, expands the capabilities available to HECC users, and reduces the complexity of administration and maintenance.

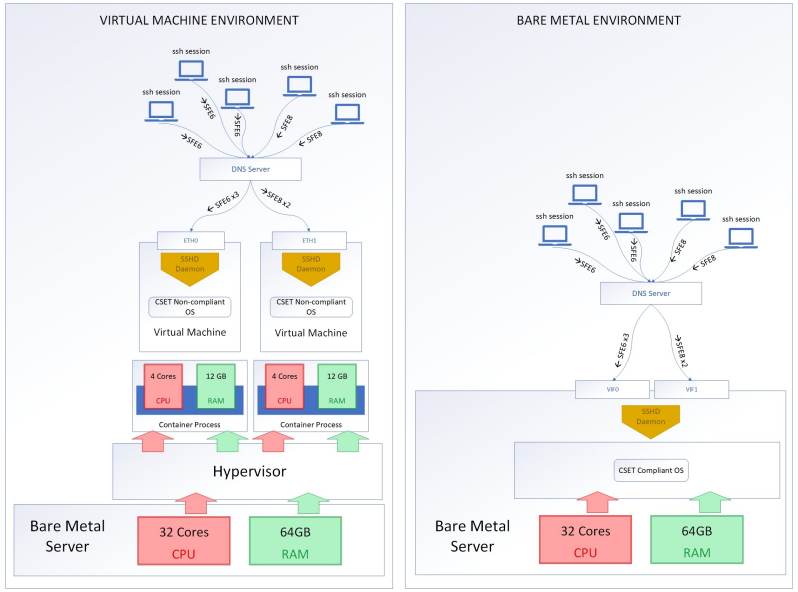


Transitioning HECC Linux systems to Red Hat Enterprise Linux 8 required significant “hands-on” attention to each of 400 systems—a challenge in getting all the systems upgraded by the mandated deadline. *Red Hat 8 logo courtesy of Red Hat Enterprise*

SFE and SUP Systems Upgraded and Enhanced

- The HECC Systems team upgraded the secure front-ends (SFEs) and Secure Unattended Proxies (SUPs) to new hardware and made them fully compliant with the Agency Security Configuration Standards (ASCS).
- The team moved the SUP systems to new hardware with an upgraded operating system, and redesigned the systems to operate within ASCS compliance constraints while maintaining their unique capabilities.
- The SFE systems were switched from virtual machines to bare metal on new hardware, which provides the advantage of being physically separated from other servers, increasing capacity and performance.
- The SFEs were changed from Red Hat to Oracle Linux, allowing them to utilize Oracle's K-Splice capability in the near future to significantly reduce the window in which unpatched vulnerabilities exist while increasing availability—both vital for bastion systems.

IMPACT: The SFEs and SUPs are critical capabilities that users rely on to access the HECC environment while shielding HPC assets from direct internet attack with a hardened least privilege security architecture.



By moving from virtual machines to bare metal, the HECC secure front-end architecture is simplified, and artificial virtual machine resource constraints are removed.

New Cluster Manager Deployed Across HECC Systems

- As part of the TOSS 4 upgrade, HECC supercomputing systems were migrated from the legacy Tempo cluster manager to HPE Cluster Manager (HPCM), which natively supports the latest HPE hardware.
- This work included the migration of:
  - Pleiades, Aitken, and Electra admin nodes to HPCM; as well as discovery of all the Pleiades supercomputer's 11,290 computational nodes and front-end nodes.
  - Aitken and Electra supercomputer nodes that comprise the Modular Supercomputing Facility (6,656 nodes).
  - Endeavour supercomputer shared memory nodes (2 nodes).
  - Lou mass storage system and its front-end systems, which house thousands of petabytes of user data for users conducting complex computational modeling and simulation for the agency's science and engineering programs and projects;
  - The Portable Batch System servers, which enable users to submit, monitor, and manage the computational jobs running on the supercomputers.
- HECC systems are now fully managed by the new HPCM provisioning system.

IMPACT: The successful upgrade to a new cluster management system allows for more efficient provisioning and management of HECC supercomputing hardware.

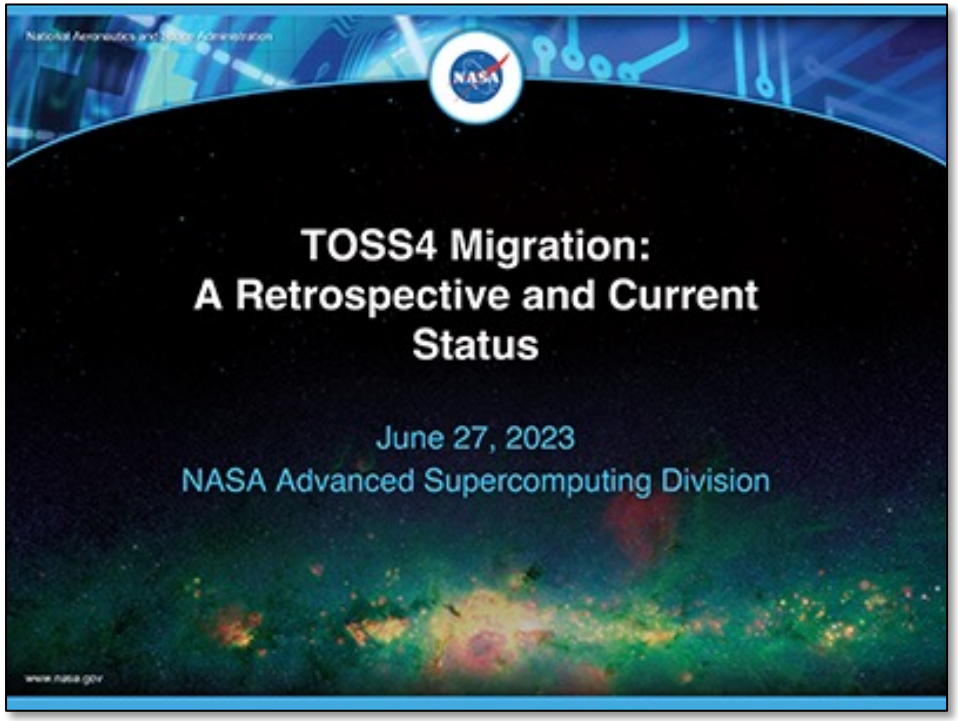


The Pleiades cluster at the NASA Advanced Supercomputing facility was a major component of the HECC upgrade to the new HPE Cluster Manager. *NASA*

Applications Team Hosts “TOSS4 Migration” User Webinar

- The HECC Application Performance and Productivity (APP) team created, hosted, and presented a user training webinar, “TOSS4 Migration: A Retrospective and Current Status” + Virtual Office Hour on Tuesday, June 27, 2023.
  - The event was conducted in a moderator format including perspectives, lessons learned, best practices, and outstanding issues on the TOSS3 to TOSS4 migration (see the May 2023 HECC monthly report).
  - The webinar addressed common support ticket topics received after the migration:
    - Using the correct HPE Message Passing Toolkit.
    - Restoring X11 functionality.
    - Intel Message Passing Interface issues.
    - pkgsrc (“package source”) related inquires.
- Twenty-nine users and staff attended, and the content was well received. The event included a Q&A session, and about a dozen questions were addressed. The webinar was recorded and posted on the HECC website for all users to access.
- The APP team will continue to monitor trends and issues experienced by the user community. Should other TOSS4 issues or best practices arise, a follow-on webinar may be developed to keep the NAS user community informed.

IMPACT: By providing the HECC userbase with best practices and solutions to common TOSS4 issues, user productivity is increased, and support staff can focus on more complicated issues.



Title slide from the TOSS4 Migration Webinar, which provided a summary of issues seen in the recent TOSS3 to TOSS4 migration from the users’ perspectives, and the resolution to those issues.

Improvements to specFEM3D Code Enables USGS Earthquake Simulations

- HECC visualization and data analysis experts improved the I/O performance of the open source “specFEM3D” code used by the U.S. Geological Survey (USGS) to simulate earthquakes.
- The code was unable to run the desired simulations due to the large number of files it was writing:
  - Each MPI rank wrote dozens of files at each time step.
  - Millions of files were produced in each run—a cumbersome and slow process that would fail due to exhausting the project’s file allocation quota on Pleiades and make post-processing impracticable.
- The HECC team added a new I/O sub-system, where:
  - Each MPI rank sends results to the I/O system, instead of writing a file.
  - Results are collected and ordered, and only two files are written per time step, regardless of the number of MPI ranks.
  - The file write time is now completely overlapped with the computation.
- With these improvements, the USGS team can now run large simulations that previously could not be run, for tens of thousands of time steps, using dozens of MPI ranks to achieve high performance.

IMPACT: HECC’s expertise in visualization and data analysis enabled these large-scale simulations to be run, leading to increased understanding of earthquake dynamics.



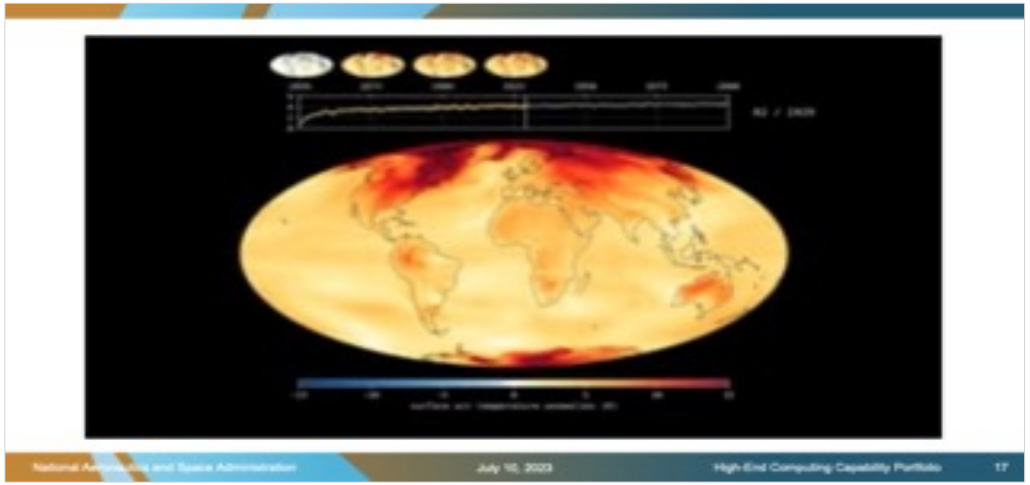
Vertical slices 40 kilometers (km) across and 45 km deep, showing components of velocity and its (Helmholtz) decomposition into P and S waves of the wavefield originating from a simulated point-source earthquake near the lower edge of the domain. *Chris Henze, NASA/Ames*

Using the NASA Chemistry Climate Model for Future Climate Simulations *

- Researchers at NASA Goddard are using global Earth-system models that include interactive chemistry, called chemistry-climate models (CCMs), to investigate the evolution of the stratospheric ozone layer and its response to the reduction of emissions of ozone depleting substances following the Montreal Protocol treaty instituted in 1989.
- The CCM uses NASA's Goddard Earth Observing System (GEOS) model, running it as a coupled atmosphere-ocean model, building off previous work producing coupled sub-seasonal to seasonal scale weather forecasts. The evaluation includes two parts:
  - A pre-industrial simulation where the oceanic and atmospheric state is forced to 1850 conditions and run for 150 years with fixed emissions.
  - A simulation that begins with 1850 conditions, but quadruples the abundance of CO_2 to simulate the response to increasing greenhouse gases.
- The equilibrium climate sensitivity—a metric that allows the team to compare the capabilities of the GEOS CCM to other climate models—was found to be 2.6 ºC, which is the calculated increase in the Earth's average surface temperature under a doubling of atmospheric CO_2.
- These simulations each used twenty 40-core CPU nodes on Pleaides, allowing the team to run a year of simulated time in a little over a day.

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

IMPACT: The diagnostic results from this effort is foundational to future work with the GEOS CCM, by establishing the credibility of the model for simulating future climate change. Future work will introduce chemistry mechanisms and impose time-varying changes in CO_2 to more realistically produce ozone & atmospheric changes.



Monthly surface air temperature anomalies from a simulation of the GEOS global Earth system model, with carbon dioxide (CO_2) concentrations quadrupled from pre-industrial levels. The anomalies are calculated with respect to a reference simulation using pre-industrial (1850) CO_2 concentrations. It illustrates how the simulated surface temperature rises and then gradually levels off in response to the increase in CO_2 concentration. *Nina McCurdy, NASA/Ames*

Scale-Resolving Simulations to Reduce Jet Noise *

- To address the Prediction Uncertainty Reduction technical challenge within NASA's Commercial Supersonic Technology (CST) project, research scientists at NASA Ames ran simulations on HECC systems to predict jet noise for single-stream asymmetric round jets at several flow conditions.
  - The goal is to provide reliable noise predictions for technical committees to approve future FAA noise regulations.
- The team performed wall-modeled large-eddy simulations (WMLES) with the Launch, Ascent, and Vehicle Aerodynamics (LAVA) computational fluid dynamics (CFD) software to predict jet acoustics for NASA's Low Boom Flight Demonstrator (LBFD).
  - They developed best practices and assessed uncertainties, strengths, and drawbacks of each simulation method; and ran validation cases with increasing complexity, such as jet-surface interaction noise, multi-stream, and chevron nozzle designs.
- Simulation results included successful prediction of jet noise and jet-surface interaction noise, and greatly improved performance, which reduced the overall simulation time by about 65x (since 2019) and the runtime from weeks to hours.

IMPACT: Increasing the output of scale-resolving simulations from a few per year to several per month gives a better understanding of the uncertainties and strengths of WMLES for jet noise predictions. Gaining confidence in the predictive capabilities of LES for jet noise is a step toward vehicle certification by analysis.



Frame from a wall-modeled large eddy simulation of a complex multi-stream nozzle for a low-boom supersonic aircraft configuration.
Gerrit-Daniel Stich, Timothy Sandstrom, NASA/Ames

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Papers

- "**The TESS-Keck Survey. XV. Precise Properties of 108 TESS Planets and their Host Stars**," M. MacDougall, et al., arXiv:2306.00251 [astro-ph.EP], June 1, 2023. *
  https://arxiv.org/abs/2306.00251
- "**Electron-Scale Current Sheets and Energy Dissipation in 3D Kinetic-Scale Plasma Turbulence with Low Electron Beta**," C. Vega, et al., arXiv:2306.01932 [physics.plasm-ph], June 2, 2023. *
  https://arxiv.org/abs/2306.01932
- "**The Magnetic, Spectroscopic, and Photometric Variability of the Wolf-Rayet Star WR55**," S. Järvinen, et al., Monthly Notices of the Royal Astronomical Society: Letters, vol.524, issue 1, published online June 7, 2023. *
  https://academic.oup.com/mnrasl/article-abstract/524/1/L21/7191848
- "**Hybrid Data-Driven Magnetofrictional and Magnetohydrodynamic Simulations of an Eruptive Solar Active Region**," A. Afanasyev, et al., arXiv:2306.05388 [astro-ph.SR], June 8, 2023. *
  https://arxiv.org/abs/2306.05388
- "**Turbulent Boundary Layer with Strong Favorable Pressure Gradient and Curvature Effects: Streamline Coordinate and Scaling Analysis**," A. Prakash, et al., arXiv:2306.5972 [physics.flu-dyn], June 9, 2023. *
  https://arxiv.org/abs/2306.05972
- "**Closing the Gap Between Observed Low-Mass Galaxy HI Kinematics and CDM Predictions**," A. Sardone, et al., arXiv:2306.07417 [astro-ph.GA], June 12, 2023. *
  https://arxiv.org/abs/2306.07417

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

Papers (cont.)

- **AIAA Aviation Forum, San Diego, CA, June 12-16, 2023.**
  - "**Minimum Trim Drag for a Three-Surface Supersonic Transport Aircraft**," S. Seraj, J. Martins. *
    https://arc.aiaa.org/doi/abs/10.2514/6.2023-3472
  - "**Combustor-Turbine Interactions by Using the Open National Combustion Code (OpenNCC) and the Glenn-HT Code**," K. Miki, A. Ameri, T. Wey, J. Moder, M. Celestina. *
    https://arc.aiaa.org/doi/abs/10.2514/6.2023-3975
  - "**Implementation and Assessment of Menter's Galilean-Invariant γ Transition Model in OVERFLOW**," B. Venkatachari, et al. *
    https://arc.aiaa.org/doi/abs/10.2514/6.2023-3533
  - "**Transition Modeling Based on the Dual N-factor Method for the CRM-NLF Wind Tunnel Configuration**," P. Paredes, et al. *
    https://arc.aiaa.org/doi/abs/10.2514/6.2023-3532
  - "**Exploring the Accuracy of RANS Simulations for Mars Entry Vehicles**," C. Pederson, M. Schoenenberger. *
    https://arc.aiaa.org/doi/abs/10.2514/6.2023-3695
  - "**Implementation and Verification of the SST-γ and SA-AFT Transition Models in FUN3D**," N. Hildebrand, et al. *
    https://arc.aiaa.org/doi/abs/10.2514/6.2023-3530
  - "**Evaluation of Transport-Equation Based Transition Models for High-Speed Boundary Layers Using OVERFLOW**," E. Vogel, et al. *
    https://arc.aiaa.org/doi/abs/10.2514/6.2023-3531
  - "**Evaluation of Limiter Functions for Supersonic Applications**," N. Ahmad, M. Park, H. Nishikawa, L. Wang, A. Elmiligui. *
    https://arc.aiaa.org/doi/abs/10.2514/6.2023-4405
  - "**Assessing Reynolds Number Effects for Flow Over a Gaussian bump using Wall-modeled LES**," P. Iyer, M. Malik. *
    https://arc.aiaa.org/doi/abs/10.2514/6.2023-3982

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Papers (cont.)

- **AIAA Aviation Forum (cont.).**
  - "**High-Fidelity Analysis of Lift+Cruise VTOL Urban Air Mobility Concept Aircraft**," Y. Liu, C. Druyor, L. Wang. * *https://arc.aiaa.org/doi/abs/10.2514/6.2023-3671*
  - "**Extension of a Viscous Cartesian Cut-Cell Solver to the Compressible RANS Equations**," A. Kleb, K. Fidkowski, J. Martins. * *https://arc.aiaa.org/doi/abs/10.2514/6.2023-3978*
  - "**Automated Unstructured Grid Adaptation on a Strut Fuel Injector at Hypervelocity Flow Conditions**," P. Drummond, et al. * *https://arc.aiaa.org/doi/abs/10.2514/6.2023-3790*
  - "**Design and Analysis of a Jet Stretcher for High-Altitude Supersonic Free Jet Testing**," B. Heberling, M.-F. Liou, H. Reising. * *https://arc.aiaa.org/doi/abs/10.2514/6.2023-4017*
  - "**Advanced Parametric Lobe Mixer Concepts for Internally Mixed Nozzles**," W. Banks. * *https://arc.aiaa.org/doi/abs/10.2514/6.2023-3469*
  - "**Advancements in Coupled Aeropropulsive Design Optimization for High-Bypass Turbofan Engines**," A. Lamkin, et al. * *https://arc.aiaa.org/doi/abs/10.2514/6.2023-3591*
  - "**Numerical Investigation of Droplet Aerobreakup and Impingement Experiments at Mach 5**," M. Viqueira-Moreira, et al. * *https://arc.aiaa.org/doi/abs/10.2514/6.2023-4251*
- "**A Mini-Neptune Orbiting the Metal-poor K Dwarf BD+29 2654**," F. Dai, et al., arXiv:2306.08179 [astro-ph.EP], June 13, 2023. * *https://arxiv.org/abs/2306.08179*
- "**Two Sub-Neptunes around the M dwarf TOI-1470**," E. González-Álvarez, et al., arXiv:2306.08516 [astro-ph.EP], June 14, 2023. * *https://arxiv.org/abs/2306.08516*

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Papers (cont.)

- "**NEOMOD: A New Orbital Distribution Model for Near Earth Objects**," D. Nesvorny, et al., arXiv:2306.09521 [astro-ph.EP], June 15, 2023. *
  https://arxiv.org/abs/2306.09521
- "**Embedding Quantum Optimization Problems using AC Driven Quantum Ferromagnets**," G. Mossi, et al., arXiv:2306.10632 [cond-mat.mes-hall], June 18, 2023. *
  https://arxiv.org/abs/2306.10632
- "**Development of the Ames Global Hyperspectral Synthetic Data Set: Surface Bidirectional Reflectance Distribution Function**," W. Wang, et al., Journal of Geophysical Research: Biogeosciences, vol. 128, issue 6, June 17, 2023. *
  https://agupubs.onlinelibrary.wiley.com/doi/full/10.1029/2022JG007363
- "**Sensitivity Analysis of Direct Numerical Simulation of a Spatially Developing Turbulent Mixing Layer to the Domain Dimensions**," J. Colmenares, et al., Journal of Verification, Validation and Uncertainty Quantification, online June 20, 2023 *
  https://asmedigitalcollection.asme.org/verification/article-abstract/doi/10.1115/1.4062770/1164062/Sensitivity-Analysis-of-Direct-Numerical?redirectedFrom=fulltext
- "**Global MHD Simulations of the Time-Dependent Corona**," R. Lionello, et al., arXiv:2306.12551 [astro-ph.SR], June 21, 2023. *
  https://arxiv.org/abs/2306.12551
- "**Time-Dependent Dynamics of the Corona**," E. Mason, et al., arXiv:2306.11956 [astro-ph.SR], June 21, 2023. *
  https://arxiv.org/abs/2306.11956

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Presentations

- "**TOI-908: A Planet at the Edge of the Neptune Desert Transiting a G-Type Star**," F. Hawthorn, et al., Monthly Notices of the Royal Astronomical Society, published online June 22, 2023. *
  https://academic.oup.com/mnras/advance-article/doi/10.1093/mnras/stad1840/7205300
- **AIAA Aviation Forum, San Diego, CA, June 12-16, 2023.**
  - "**Simulation of a Quadrotor Urban Air Taxi Hovering Above a Rooftop Edge**," D.-G. Caprace, P. Ventura Diaz, S. Yoon.
    https://arc.aiaa.org/doi/abs/10.2514/6.2023-4281
  - "**Multi-Fidelity Computational Analysis of a Quiet Single-Main Rotor Helicopter for Air Taxi Operations**," P. Ventura Diaz, et al.
    https://arc.aiaa.org/doi/abs/10.2514/6.2023-3669
  - "**Computational Study of Low-Speed Boundary-Layer Laminar-Turbulent over a 30-Degree Swept Plate in a Channel**," M. Denison, J. Smith, J. Eppink.
    https://arc.aiaa.org/doi/abs/10.2514/6.2023-3272
  - "**Aerodynamic Simulations for Complex Geometries Using Automatically Generated Structured Overset Meshes**," A. Chuen, et al.
    https://arc.aiaa.org/doi/abs/10.2514/6.2023-3602
  - "**Microjet Angle Sensitivity for Active Flow Control on Multi-Element High-Lift Systems**," J. Koch, J. Housman, S. Hosseini.
    https://arc.aiaa.org/doi/abs/10.2514/6.2023-4307
  - "**Automatic Runtime Scheduling Via Directed Acyclic Graphs for CFD Applications**," H. Torres, S. Murman.
    https://arc.aiaa.org/doi/abs/10.2514/6.2023-3426
  - "**Anisotropic Mach Cone Aligned Mesh Adaptation for Low Boom Simulations**," C. Ashby, J. Housman, J. Duensing.
    https://arc.aiaa.org/doi/abs/10.2514/6.2023-4333

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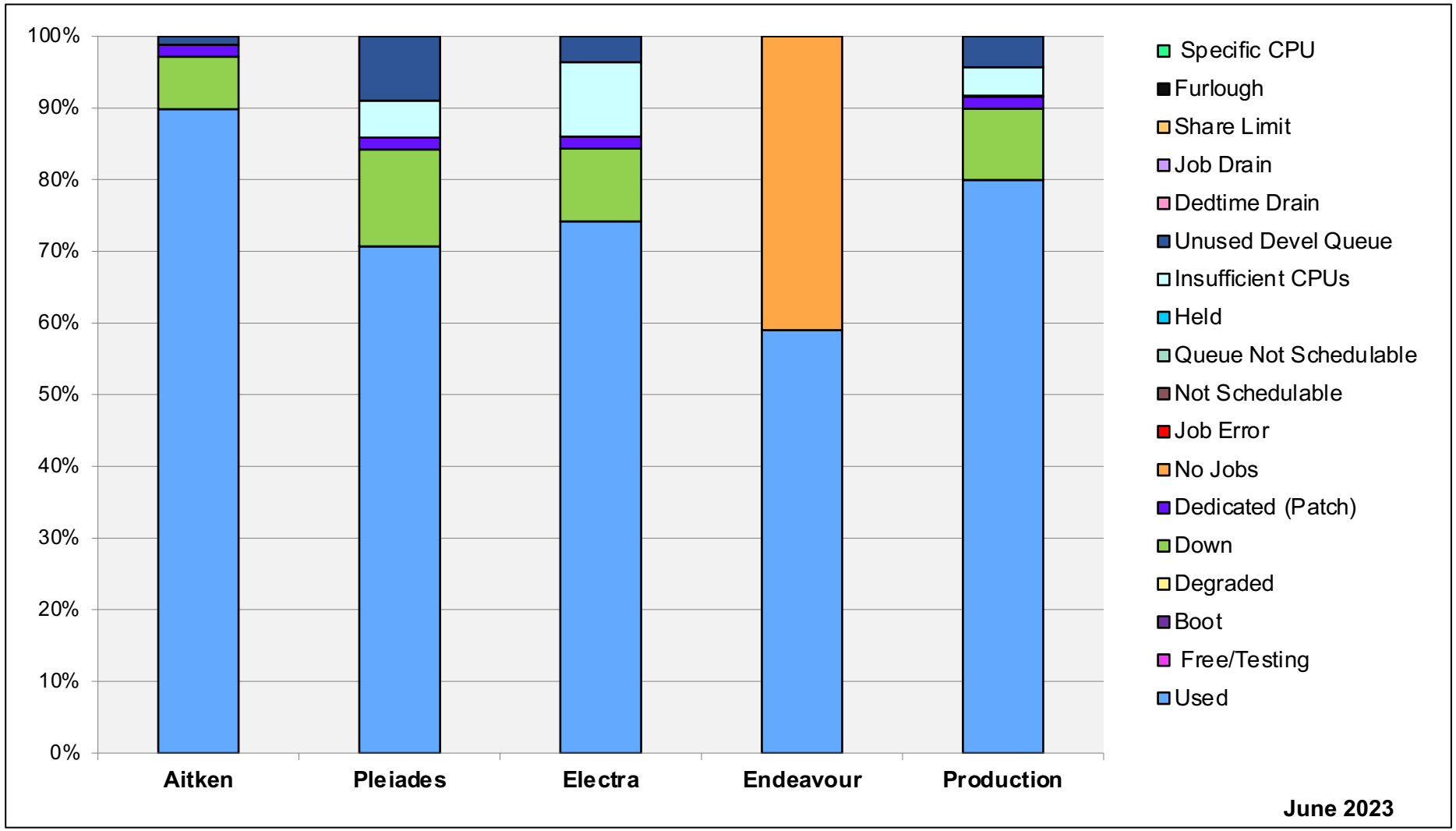
News and Events

- **Eye in the Sky with AI: USCB Initiative Aims to Pulverize Space Threats Using NVIDIA RTX**, *NVIDIA Blog*, June 9, 2023—A team from the University of California, Santa Barbara is developing more practical approaches to planetary defense called PI-Terminal Planetary Defense. Several of their simulations are accomplished using the NASA Advanced Supercomputing facility at NASA Ames.
  https://blogs.nvidia.com/blog/2023/06/09/planetary-defense-rtx/

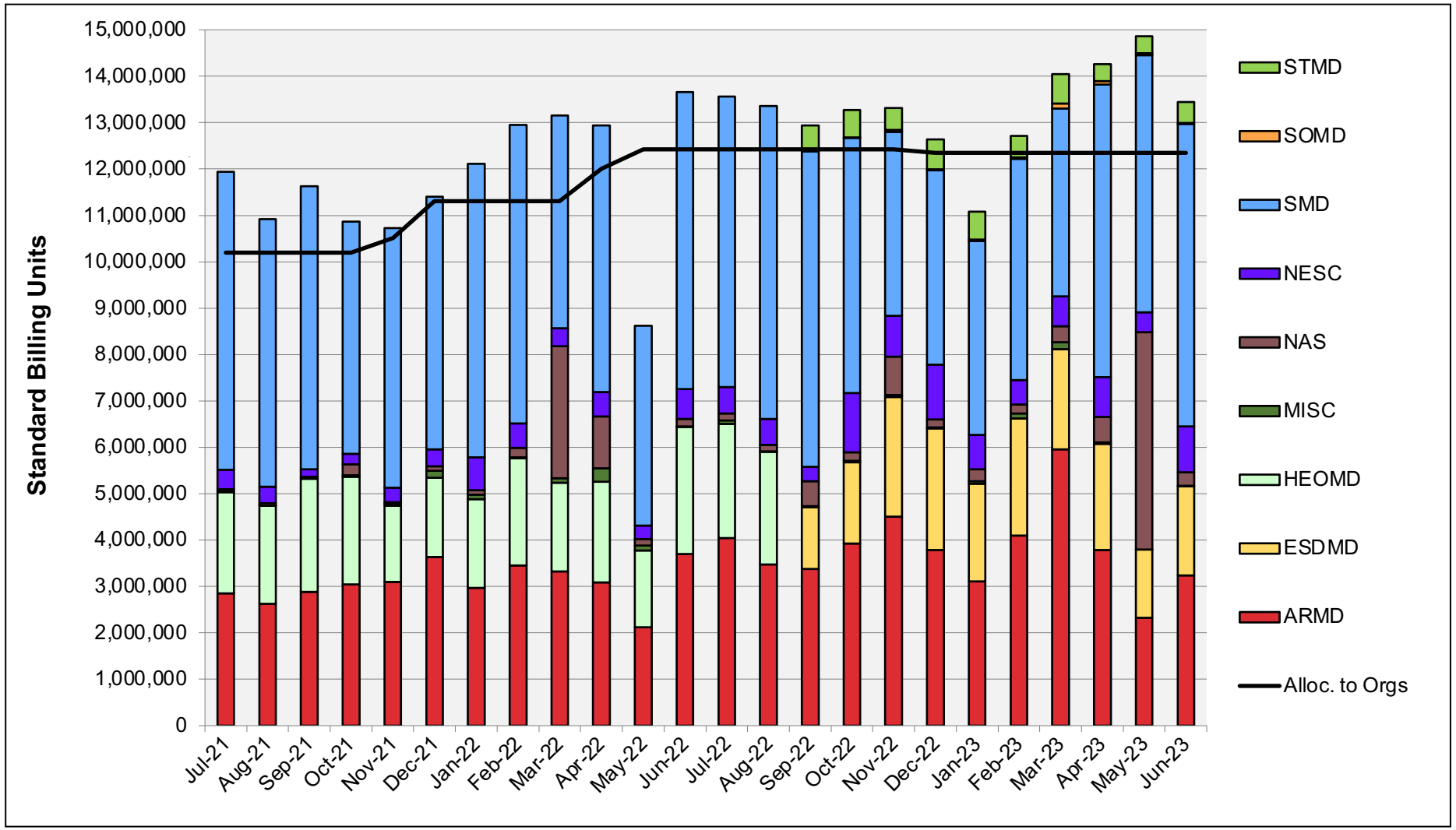
News and Events: Social Media

- **Coverage of NAS Stories**
  - AIAA Aviation Forum Attendance:
    - NAS Division: Twitter 17 retweets, 40 likes, ~4.8k views.

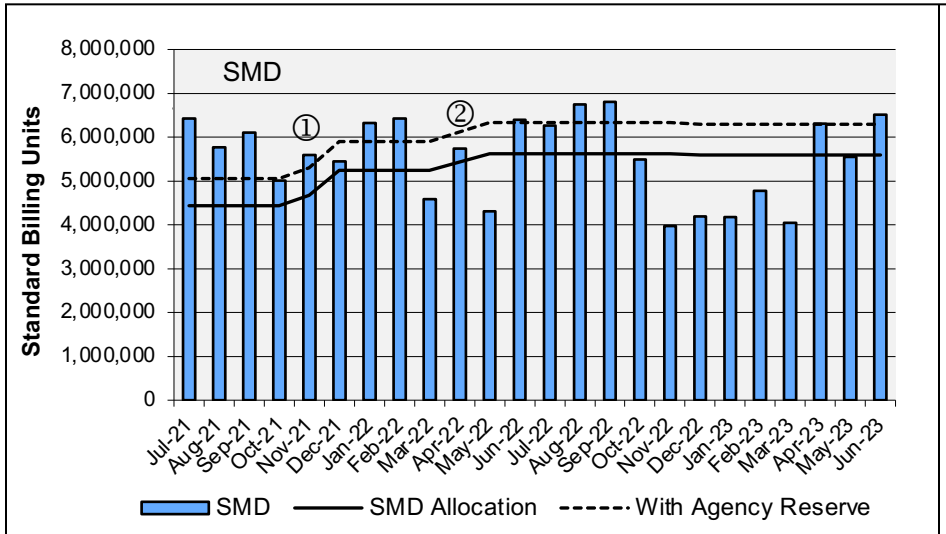
HECC Utilization

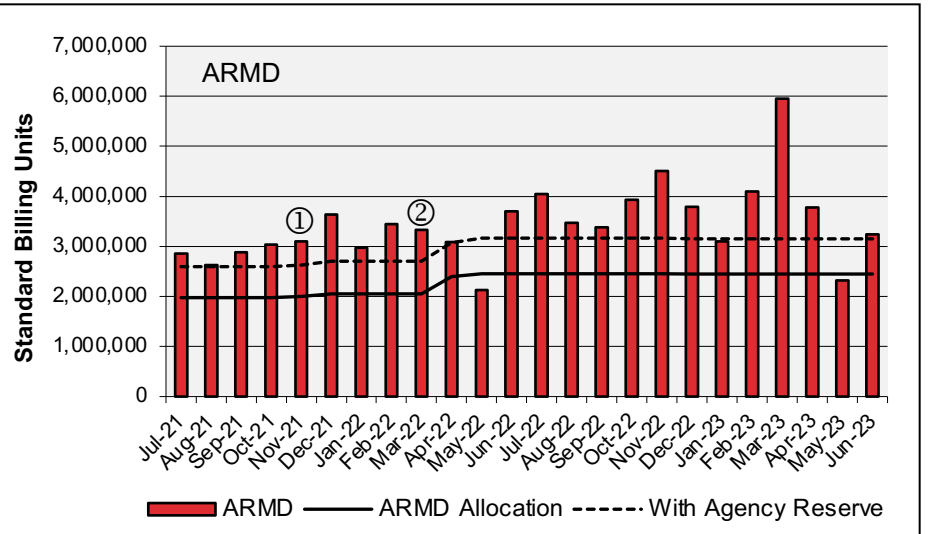


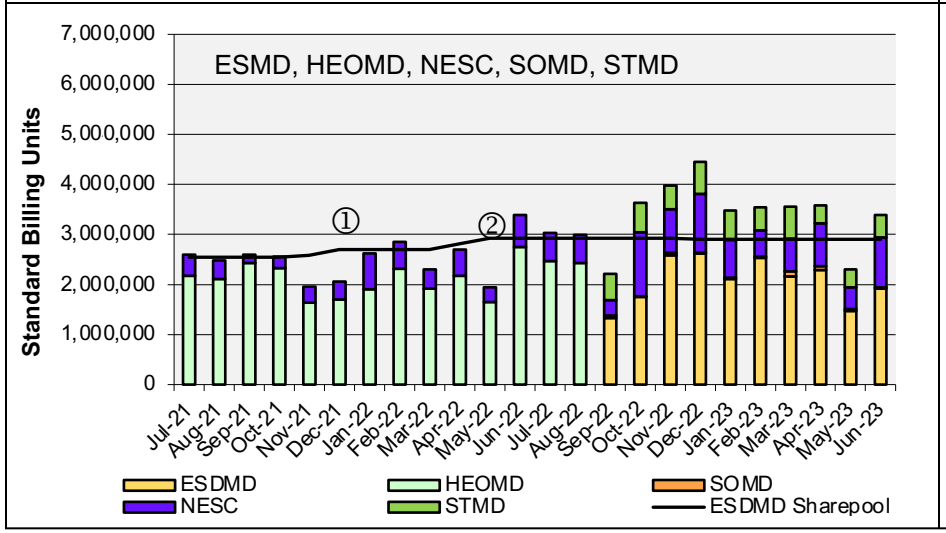
HECC Utilization Normalized to 30-Day Month



HECC Utilization Normalized to 30-Day Month



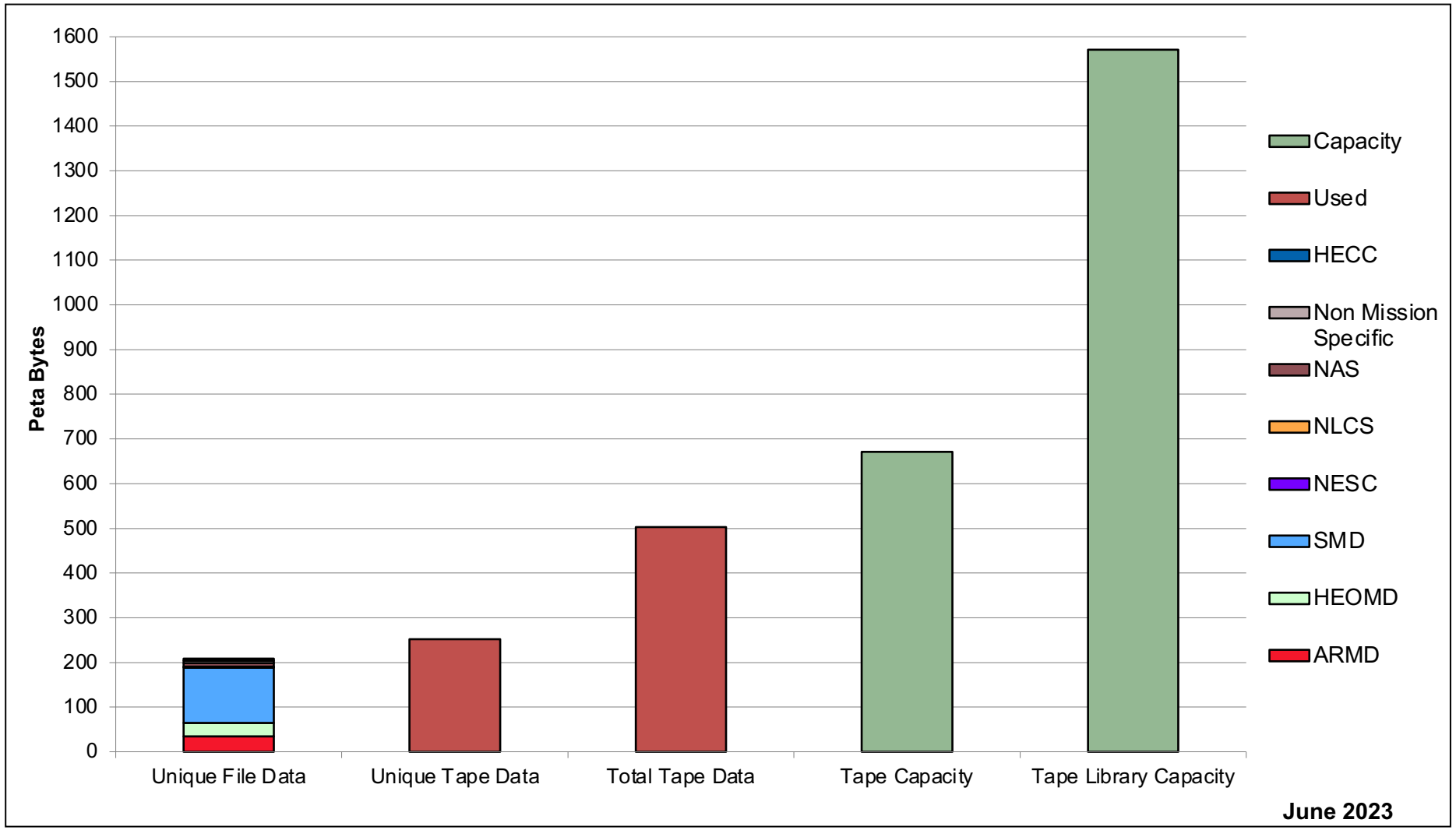




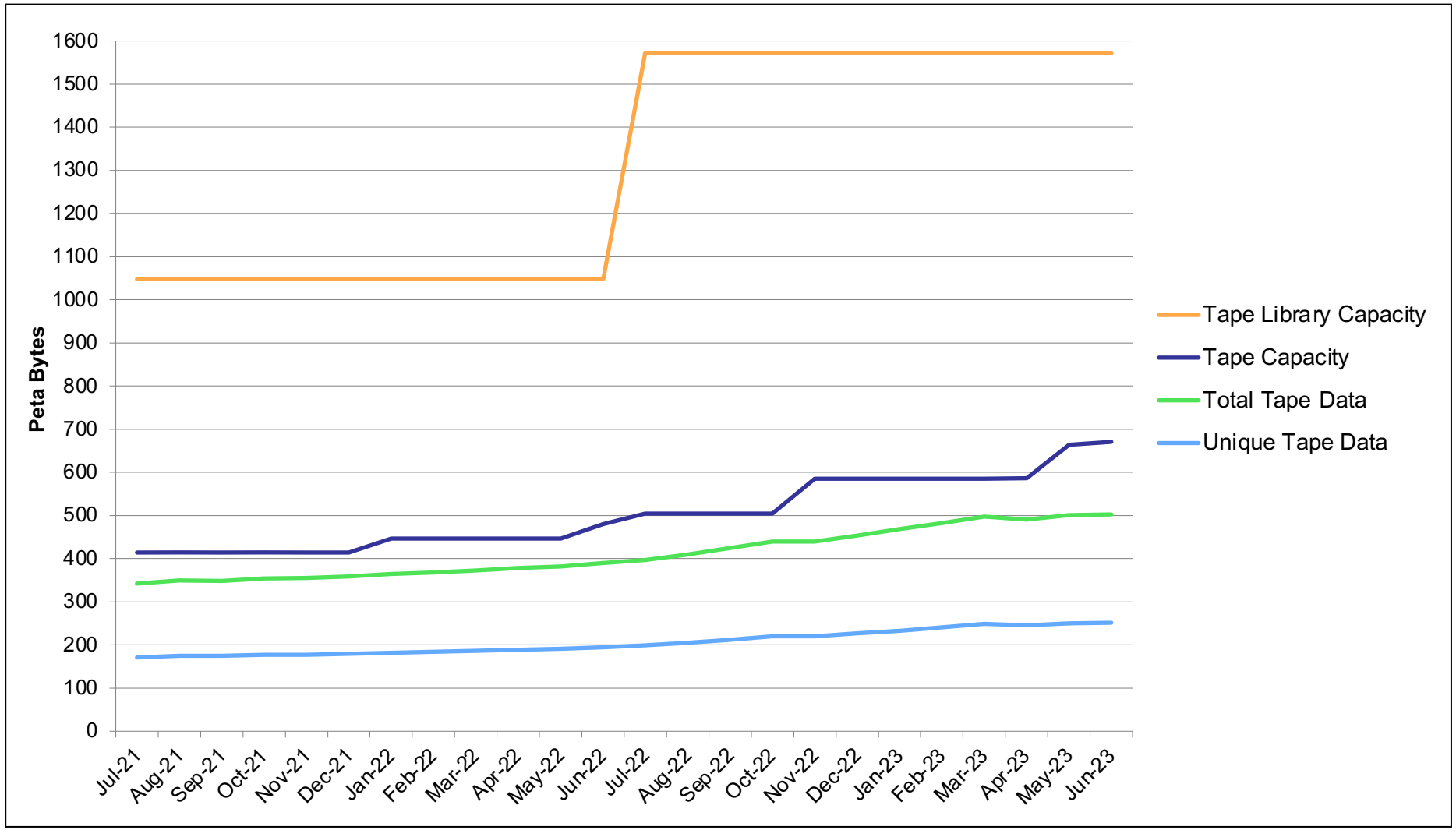
① 4 Rome Apollo Racks added to Aitken

② 4 Rome Apollo Racks added to Aitken

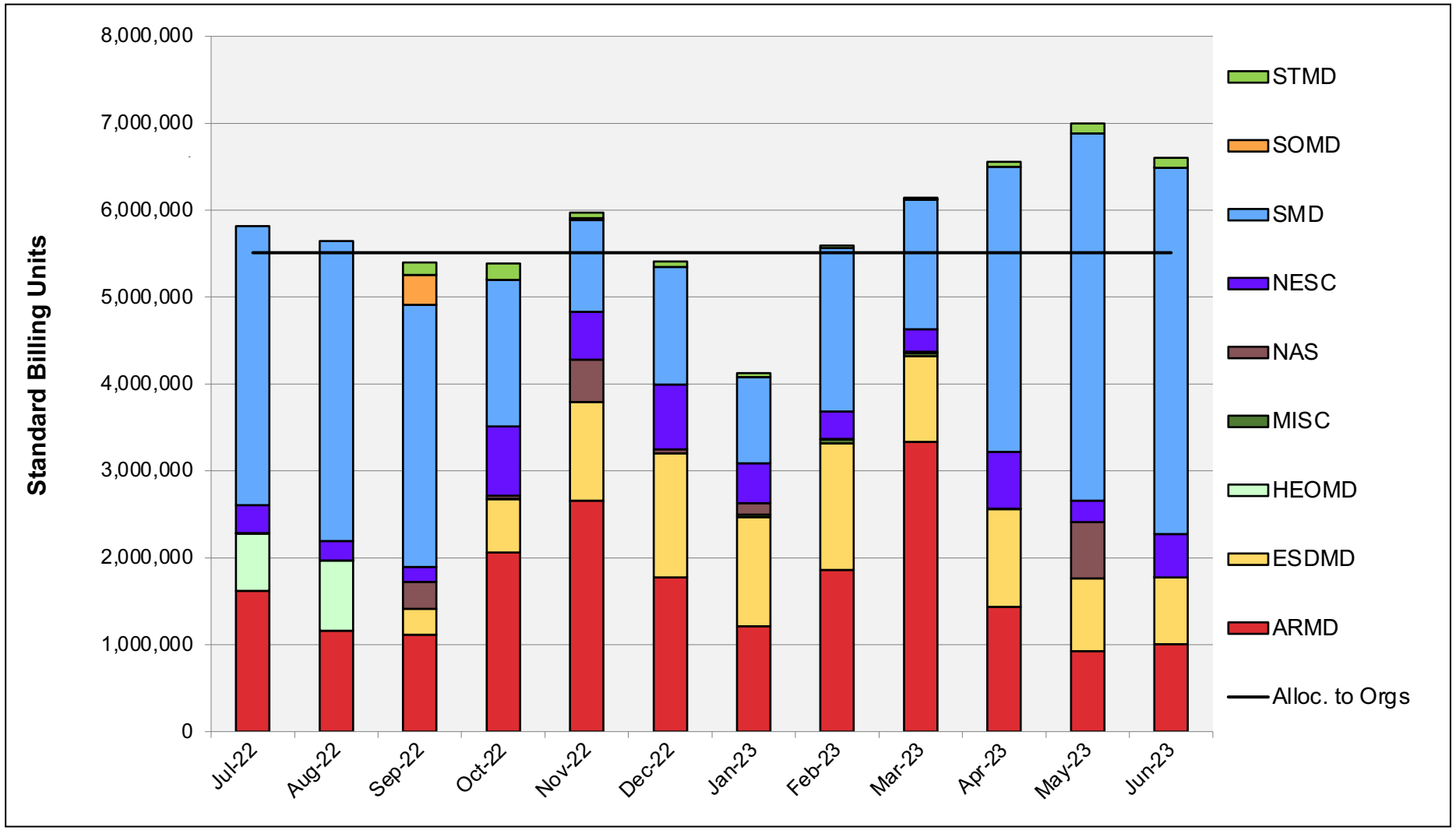
Tape Archive Status



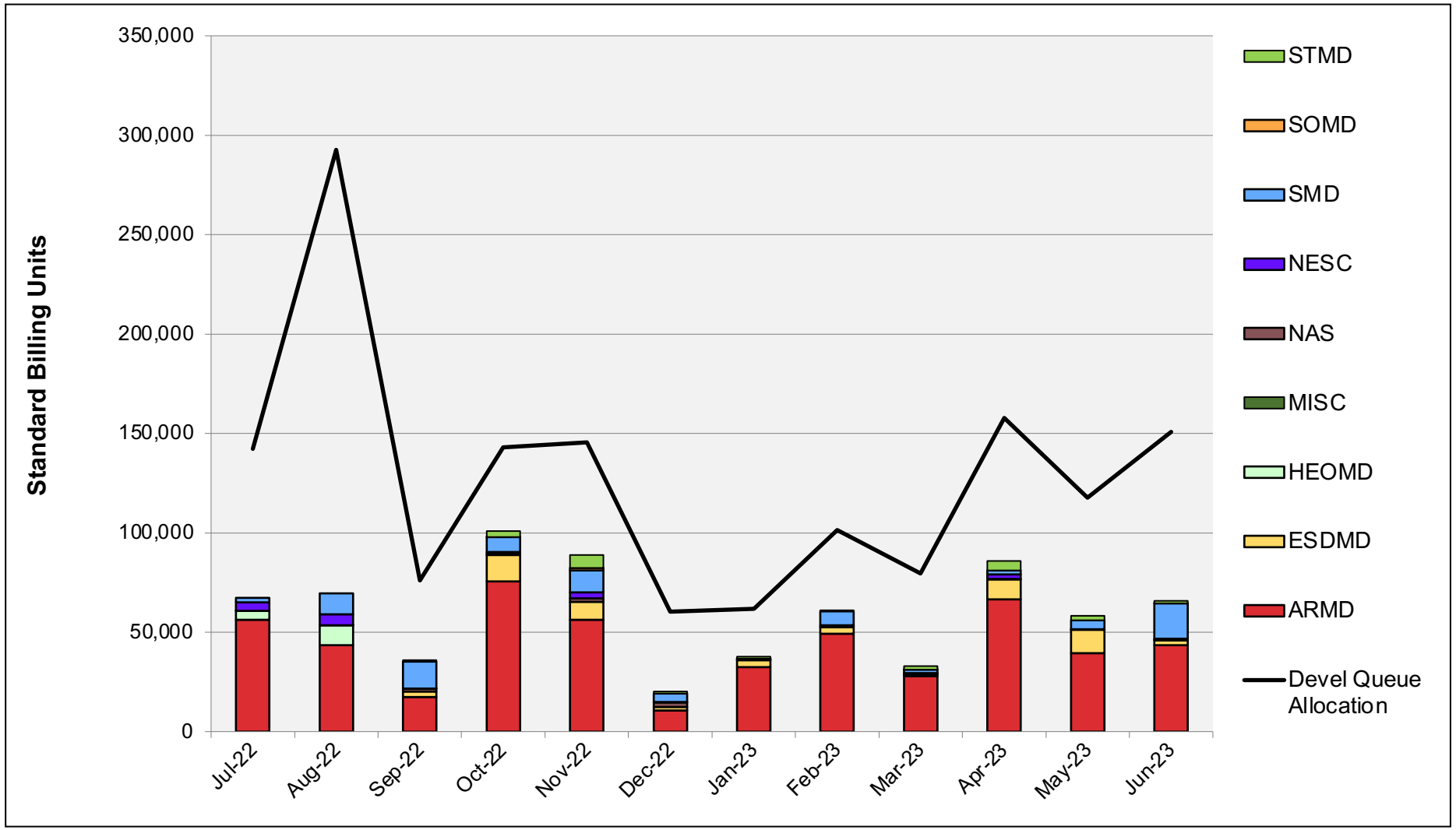
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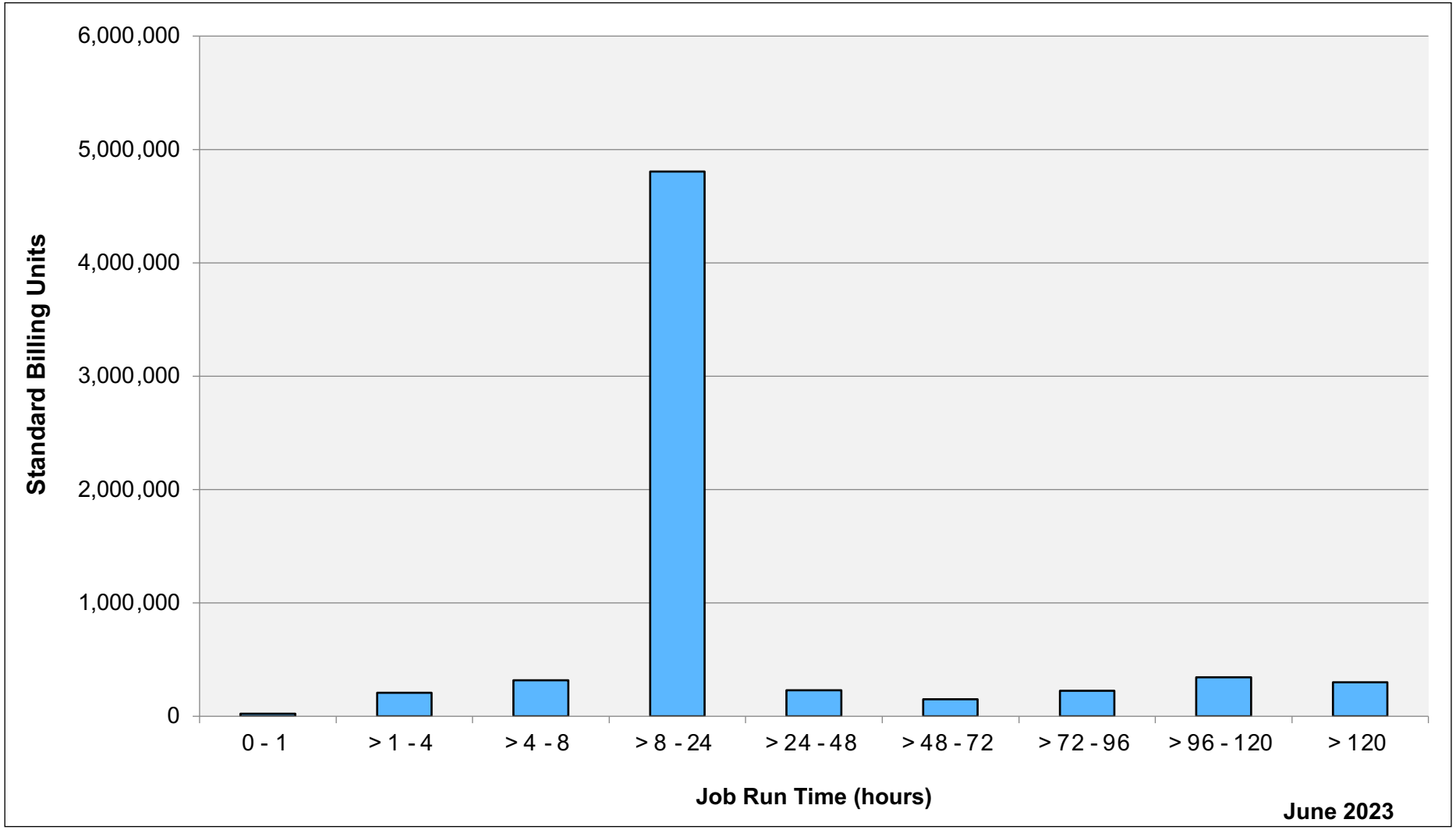
Aitken: SBUs Reported, Normalized to 30-Day Month



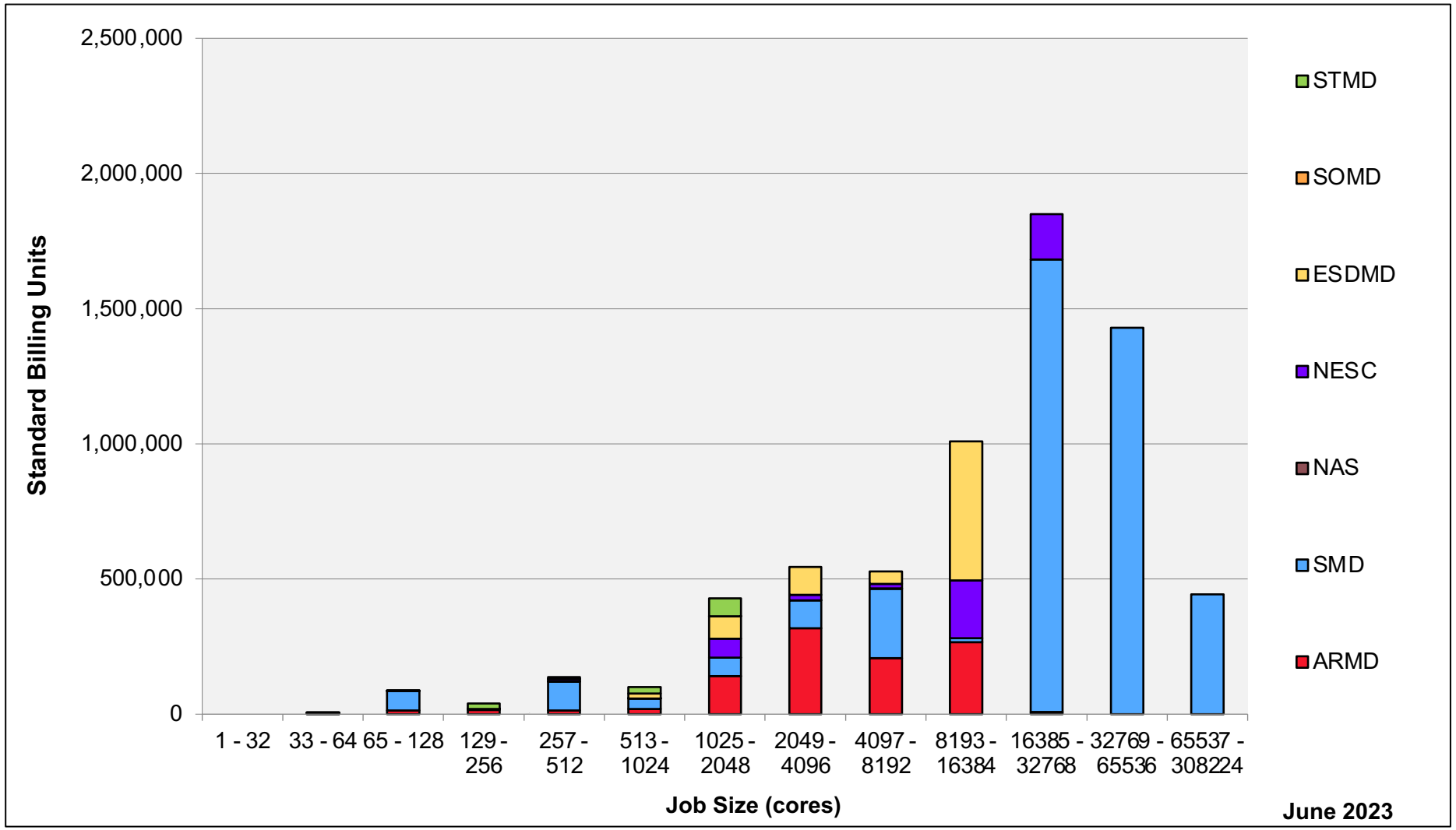
Aitken: Devel Queue Utilization



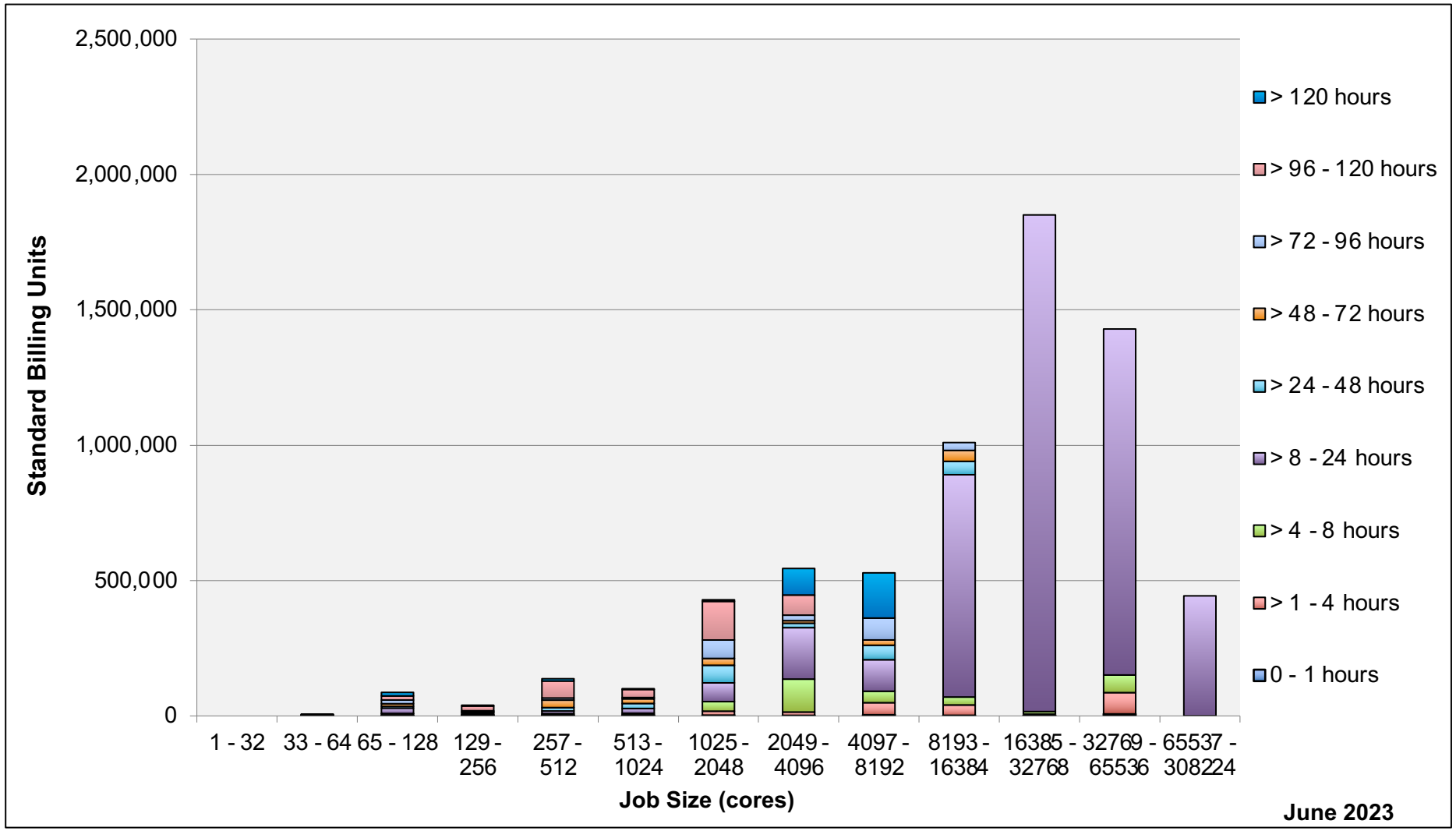
Aitken: Monthly Utilization by Job Length



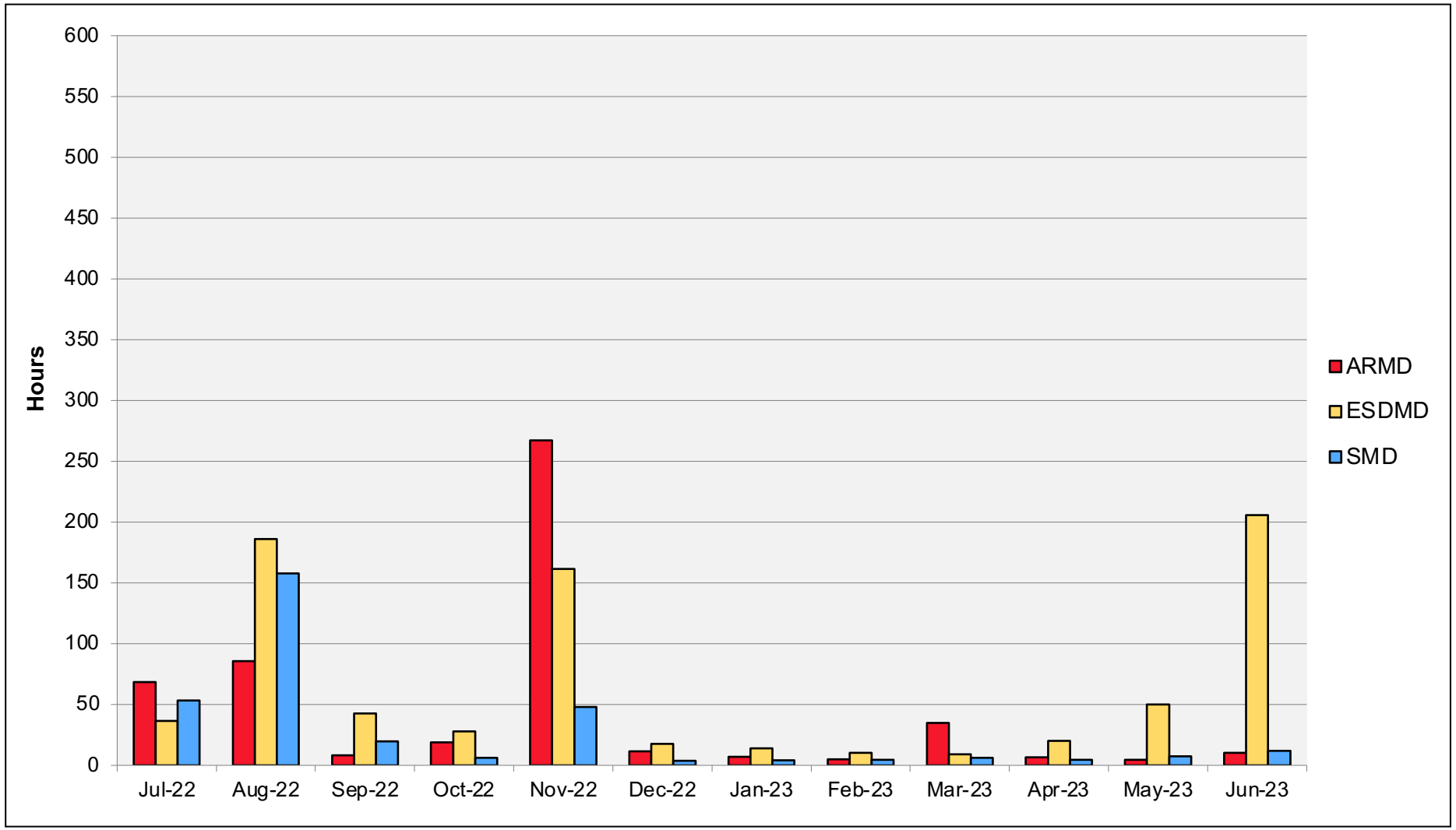
Aitken: Monthly Utilization by Job Size



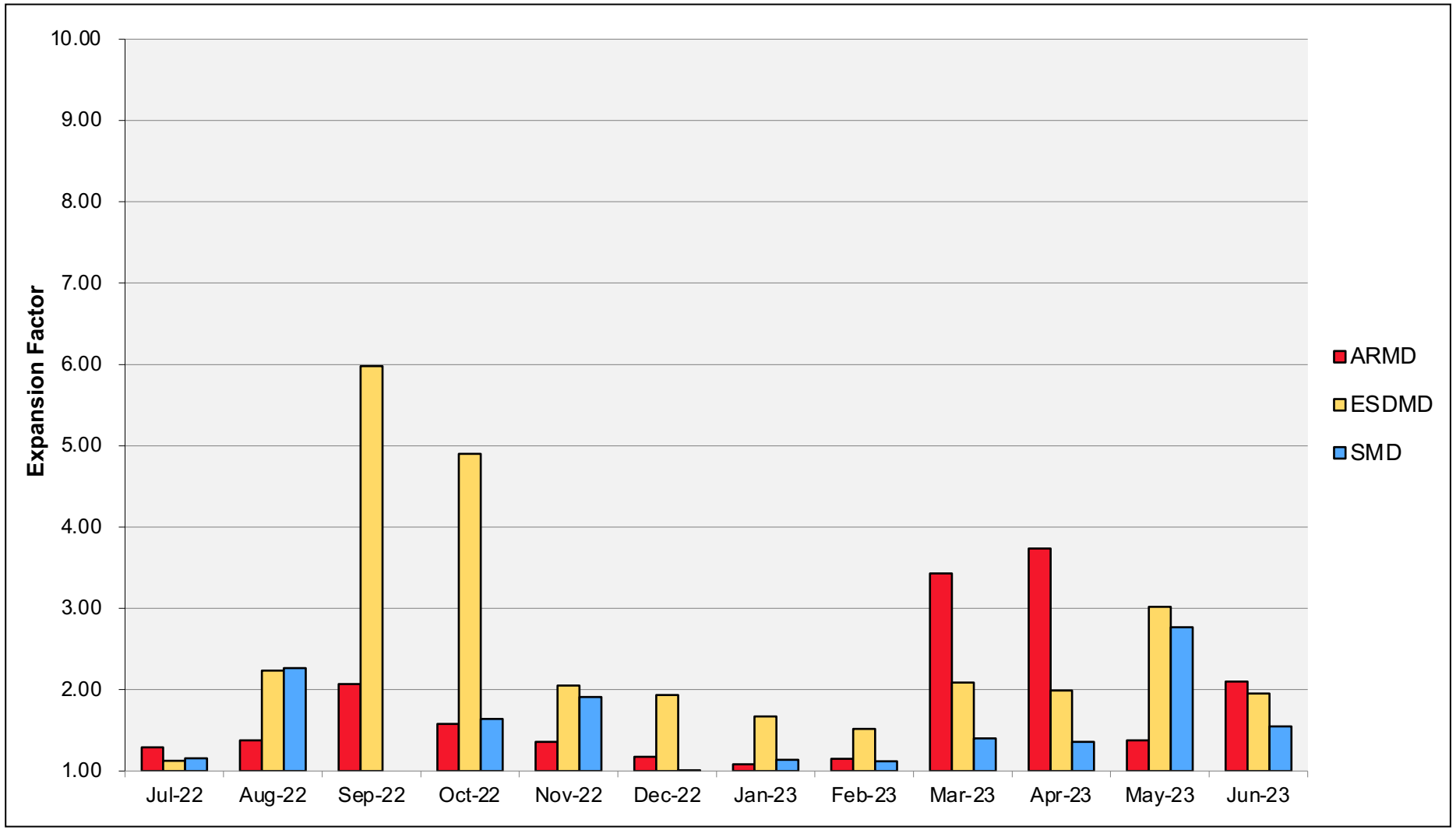
Aitken: Monthly Utilization by Size and Length



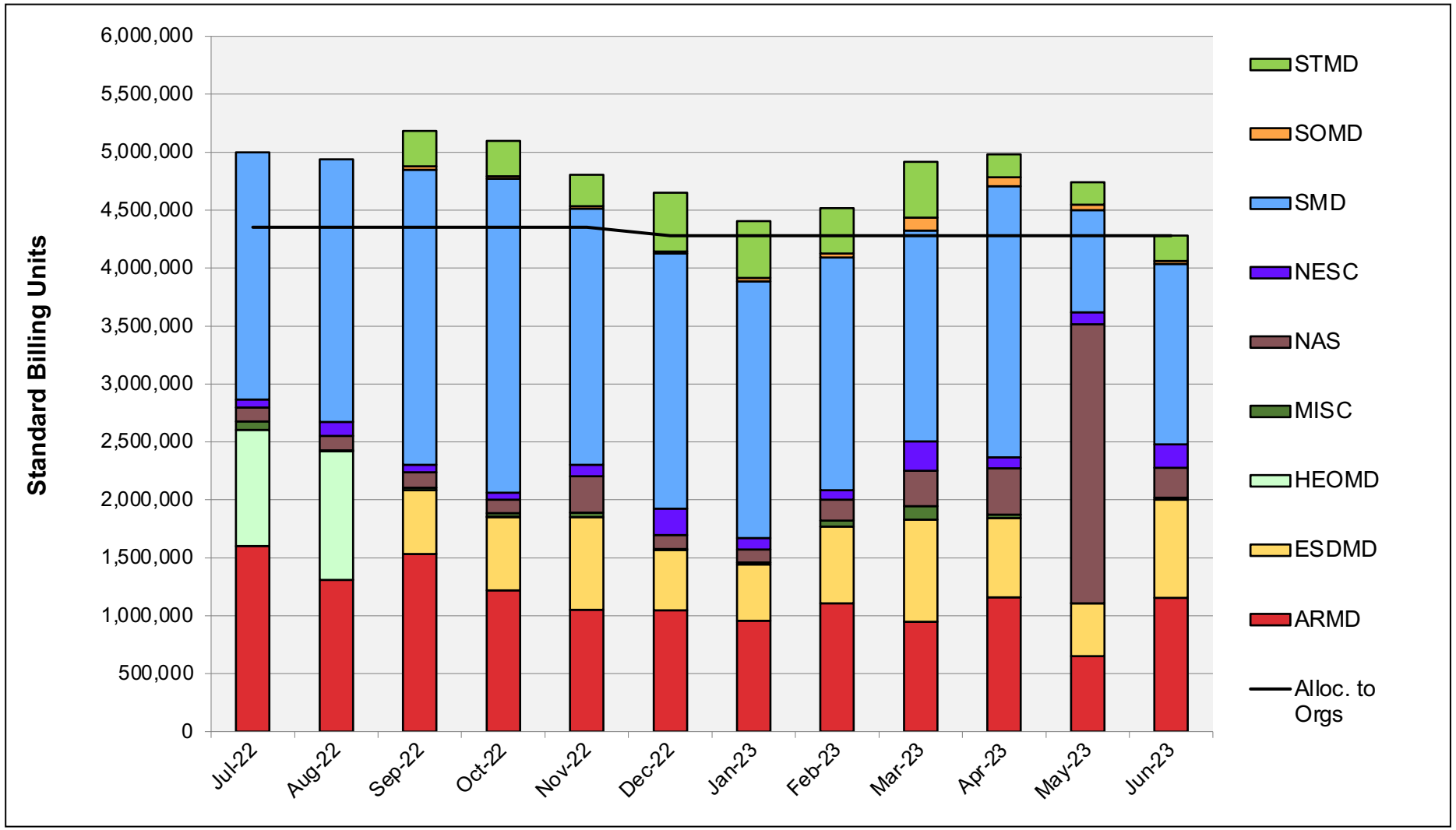
Aitken: Average Time to Clear All Jobs



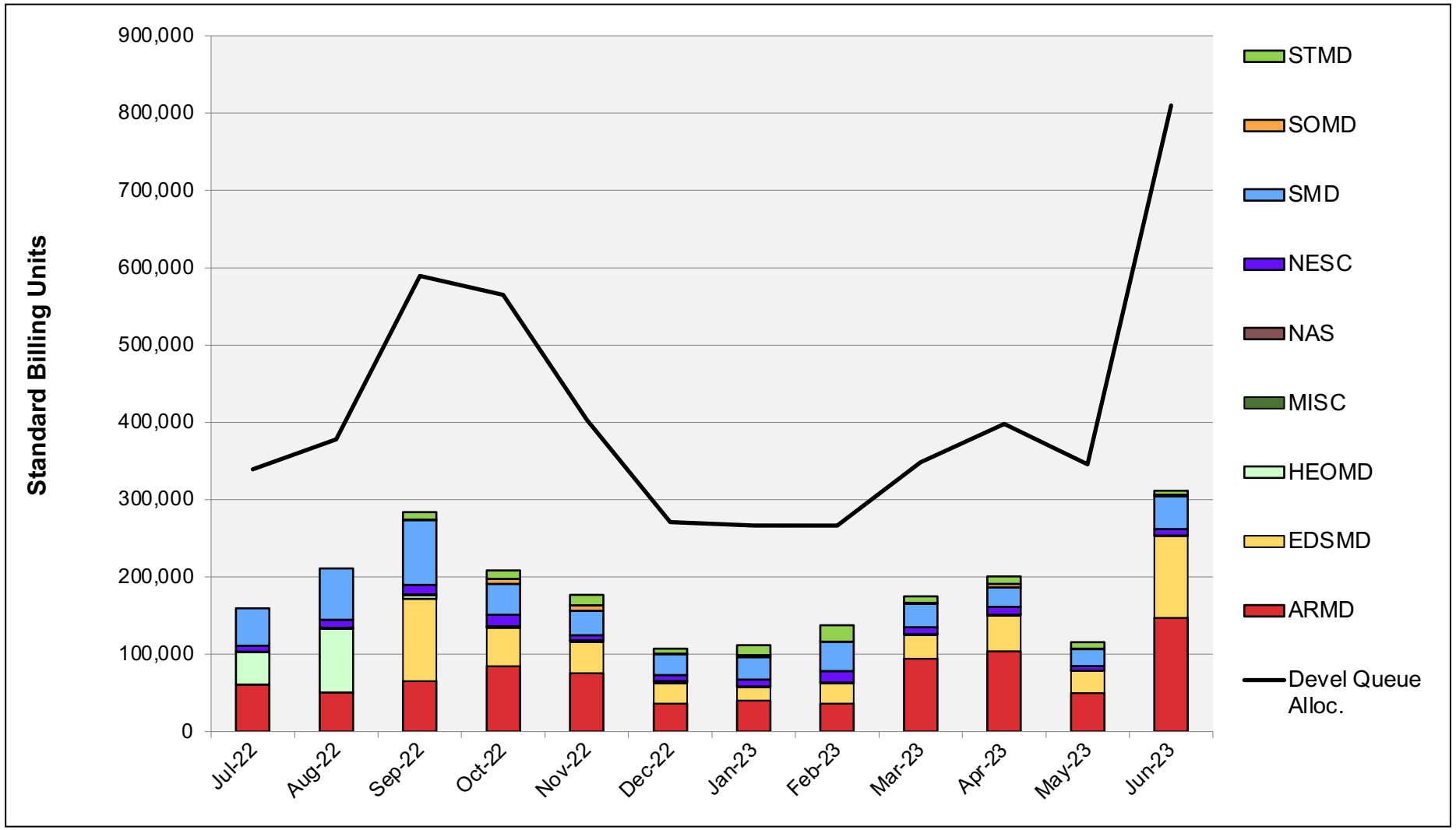
Aitken: Average Expansion Factor



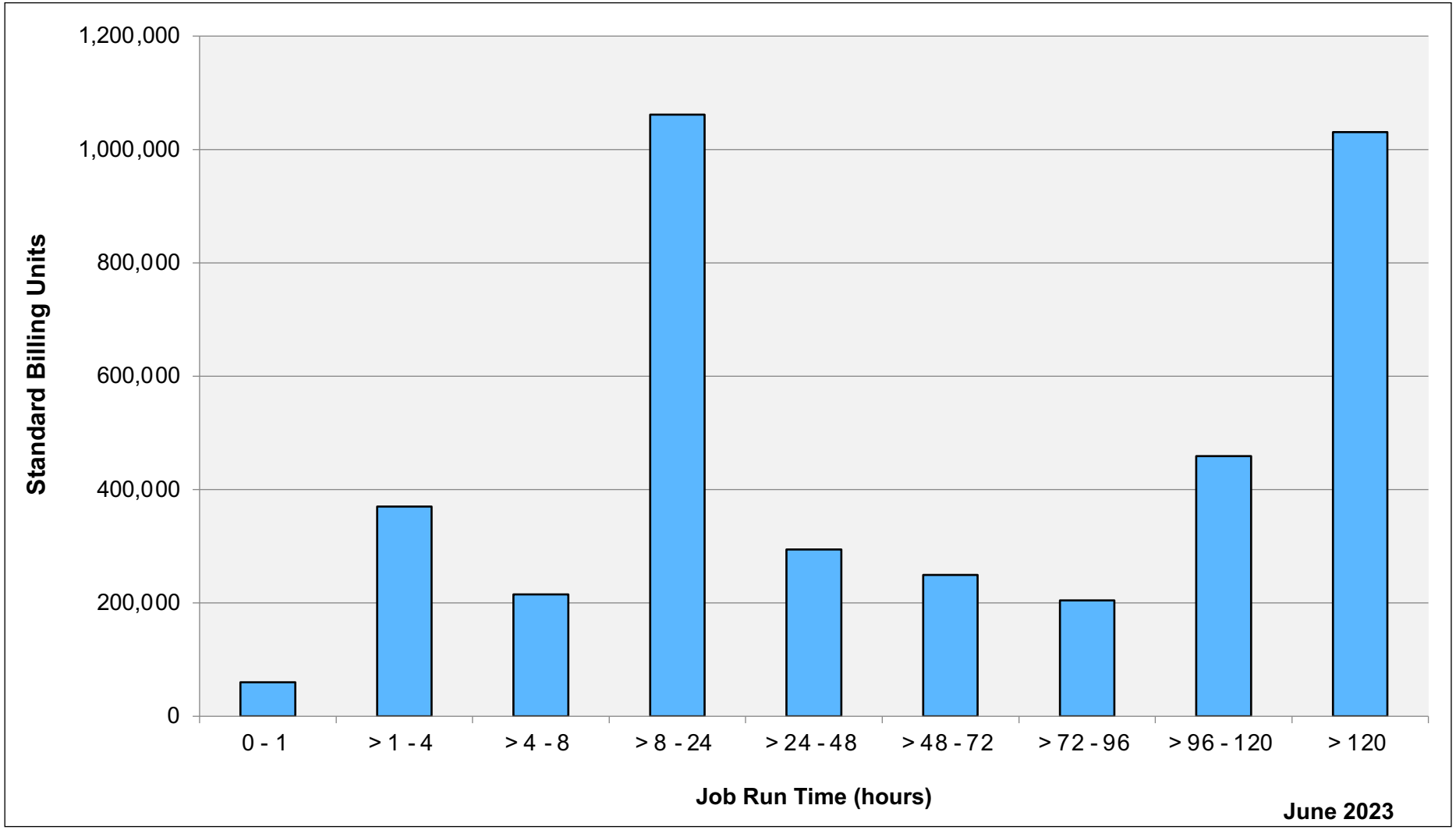
Pleiades: SBUs Reported, Normalized to 30-Day Month



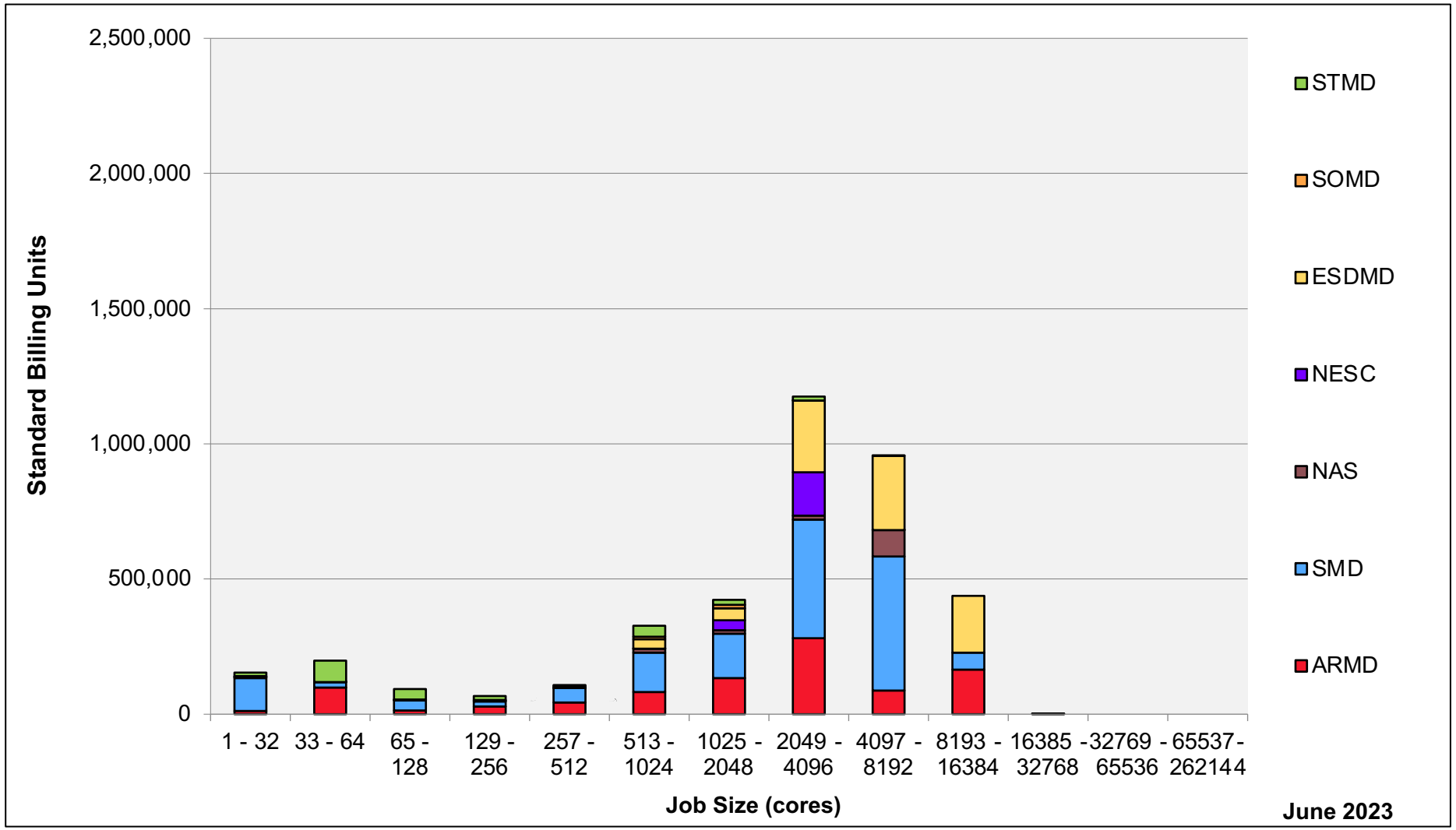
Pleiades: Devel Queue Utilization



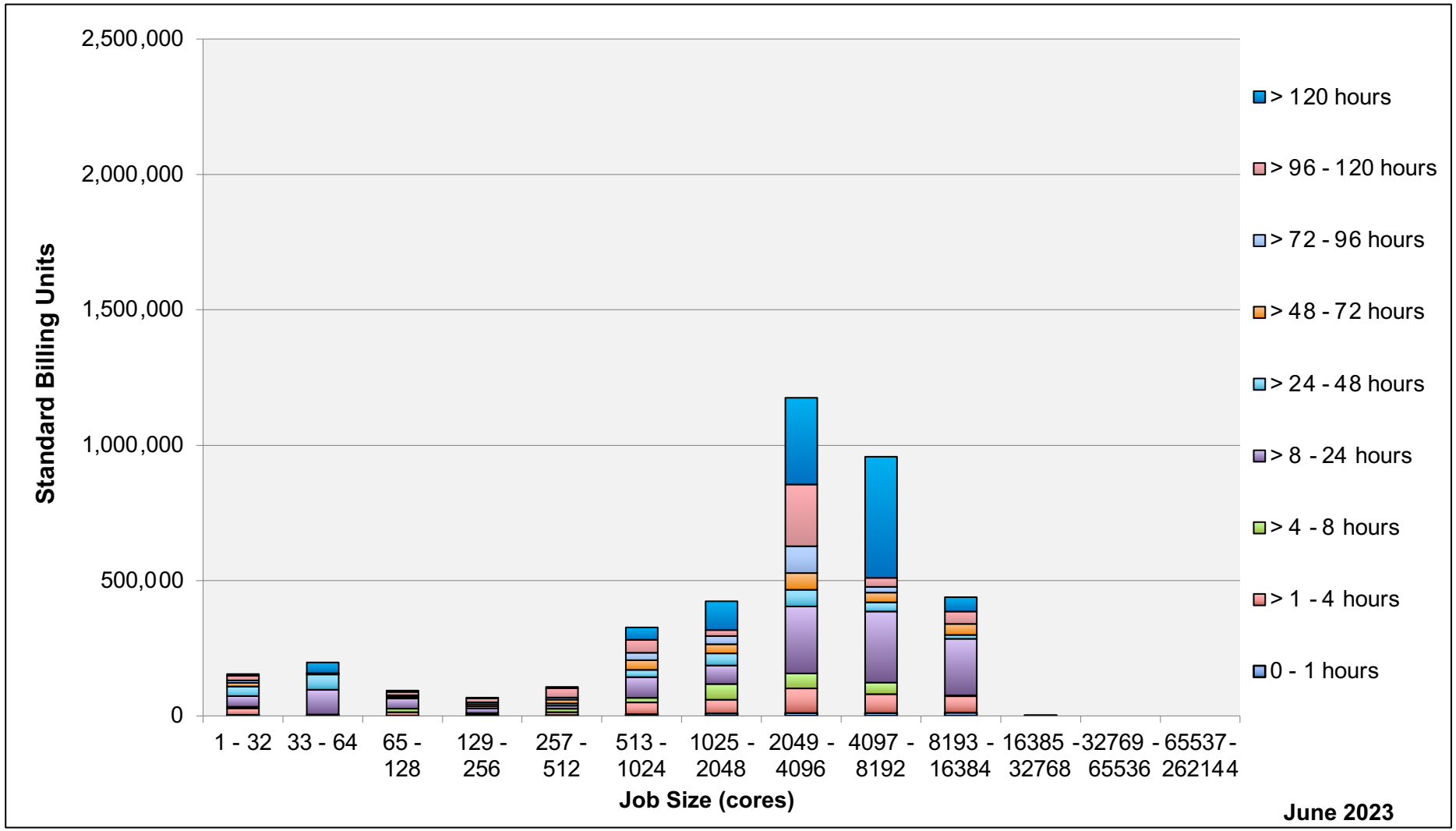
Pleiades: Monthly Utilization by Job Length



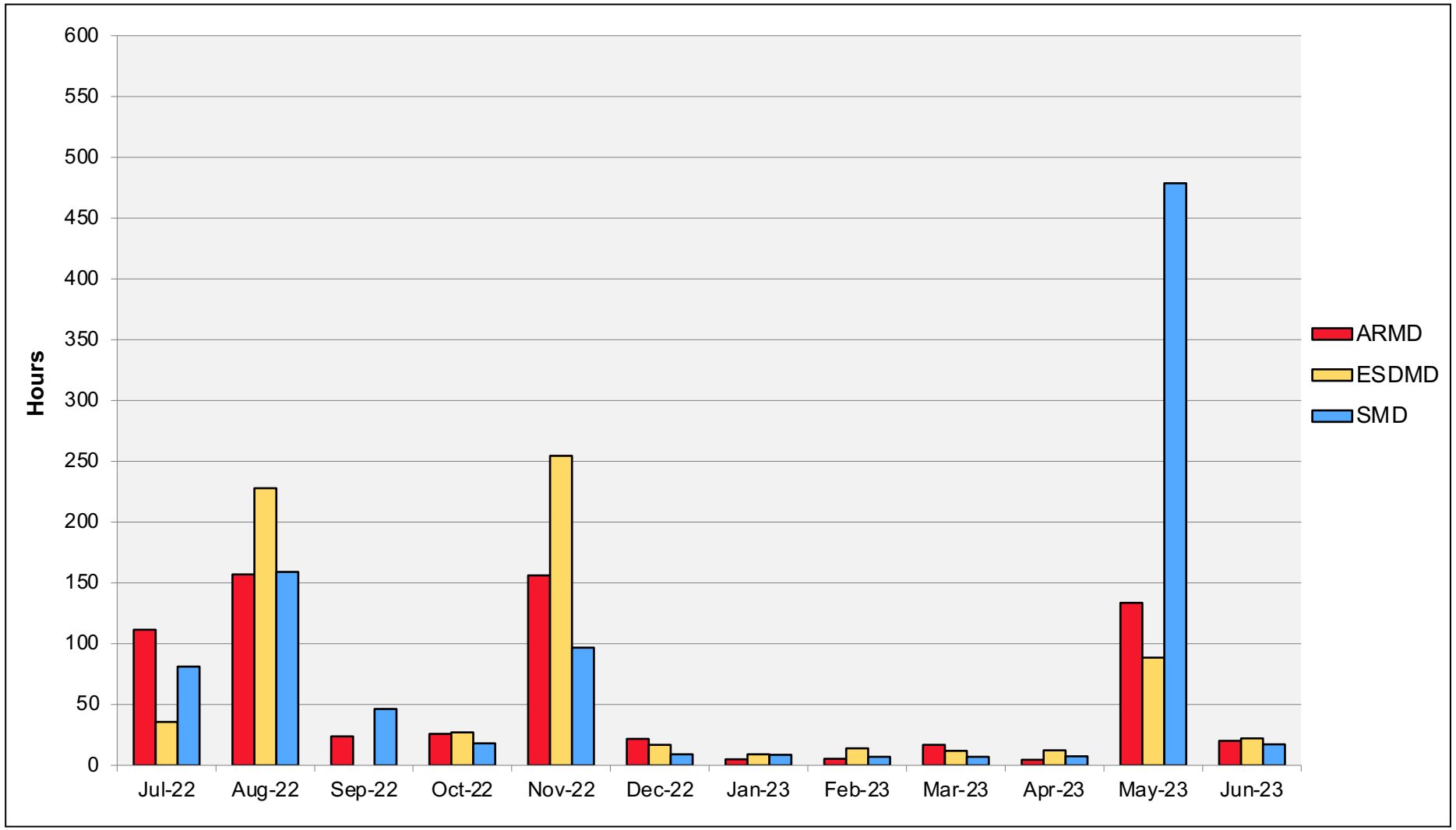
Pleiades: Monthly Utilization by Job Size



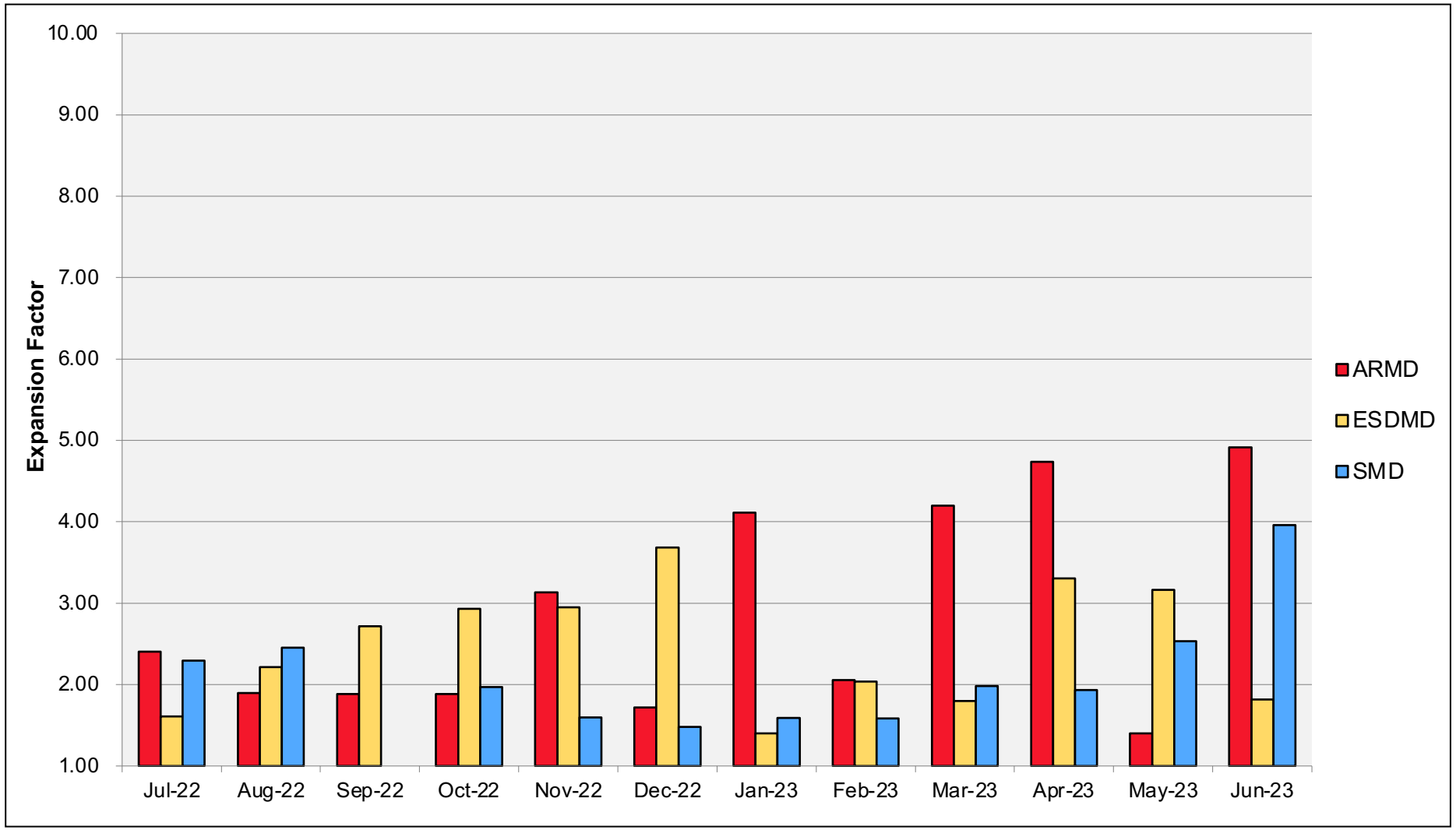
Pleiades: Monthly Utilization by Size and Length



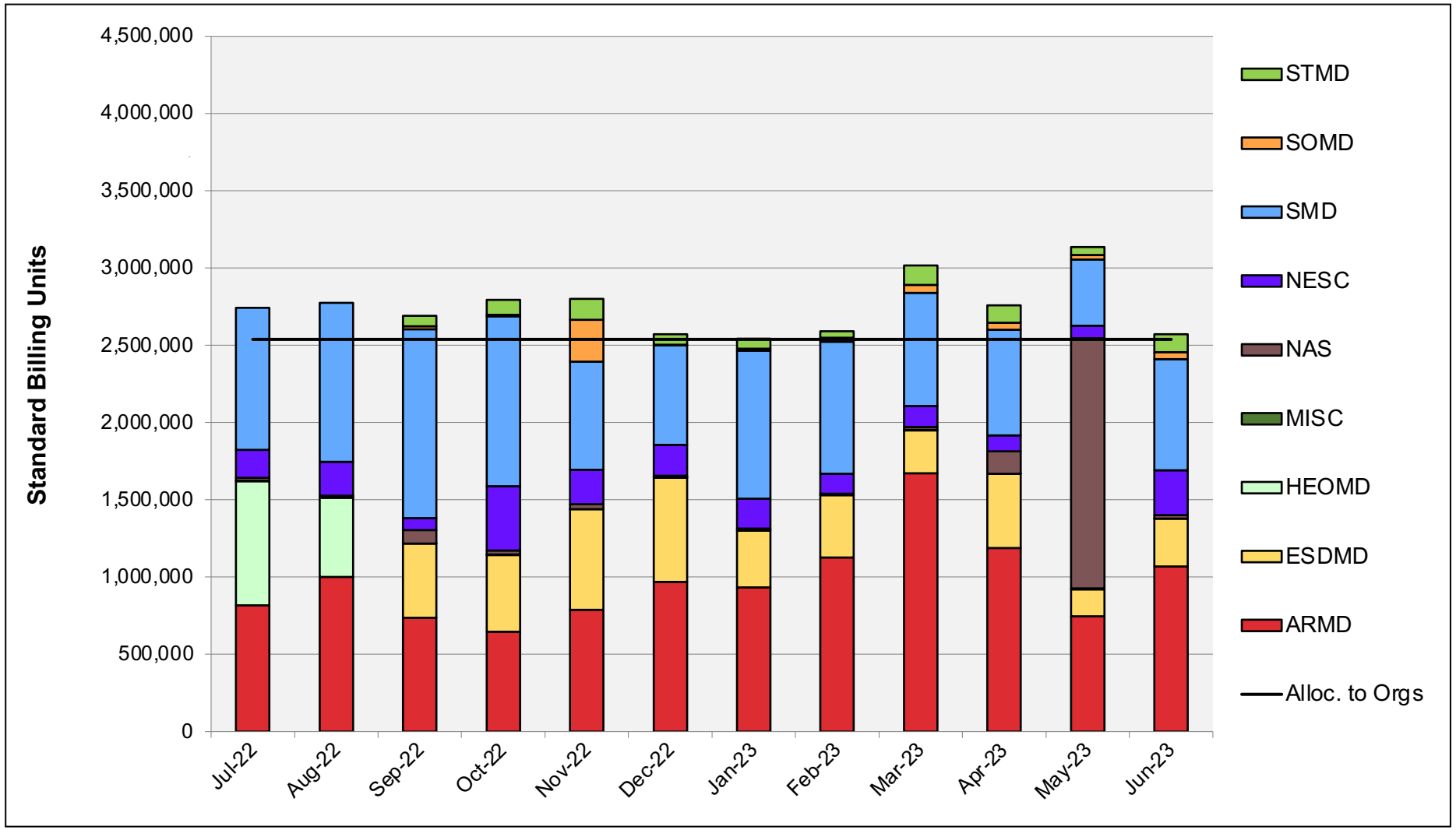
Pleiades: Average Time to Clear All Jobs



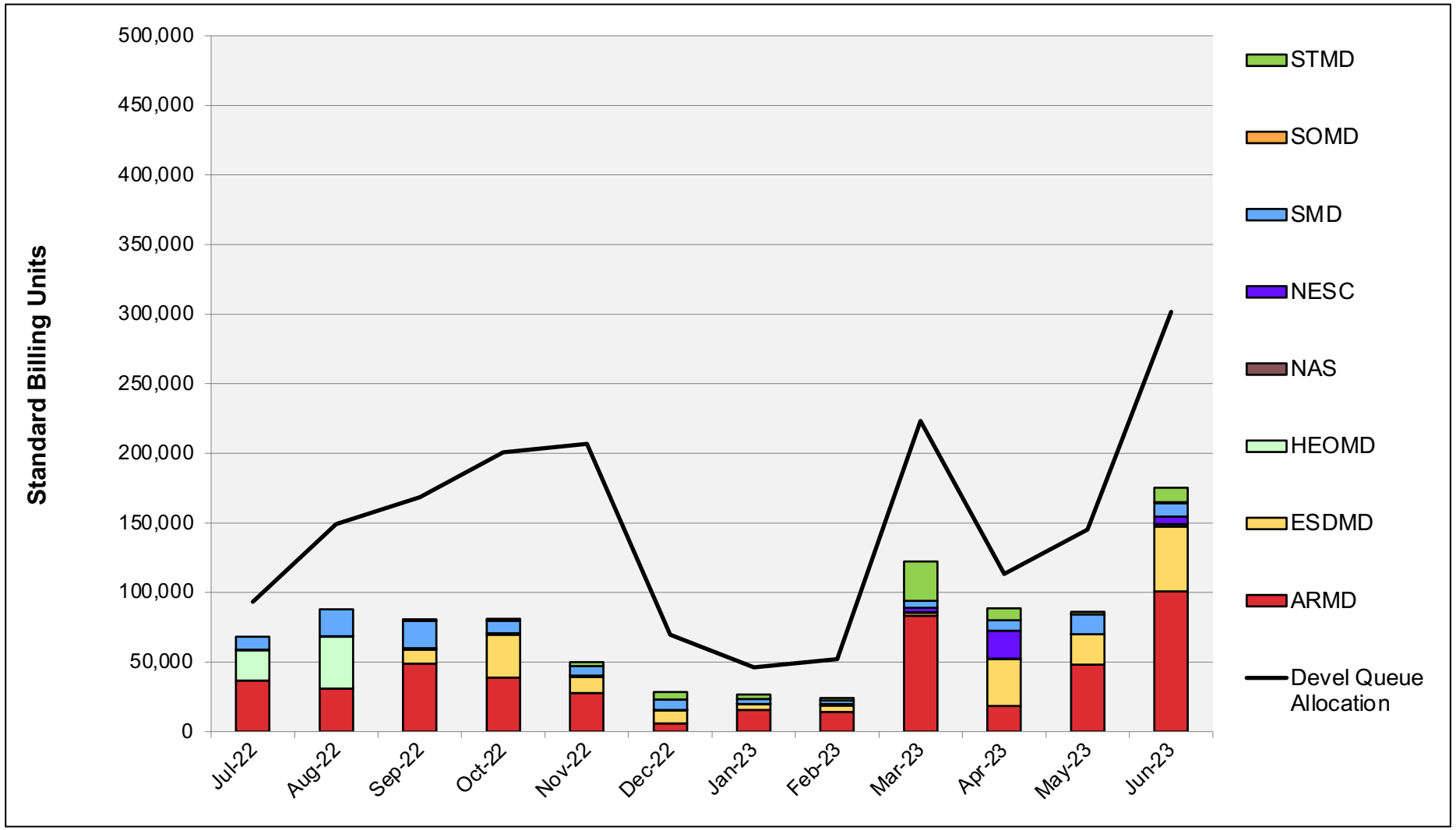
Pleiades: Average Expansion Factor



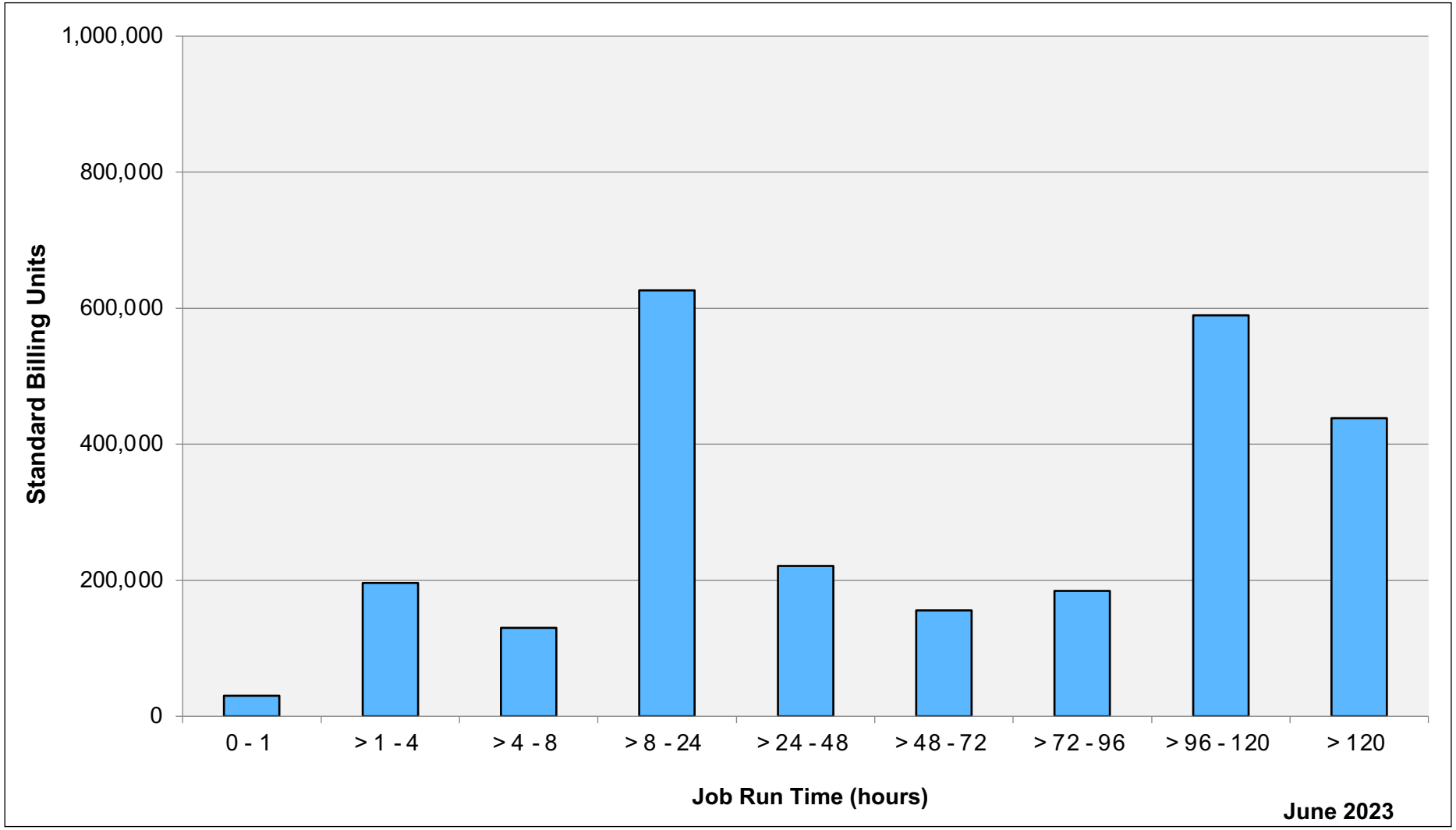
Electra: SBUs Reported, Normalized to 30-Day Month



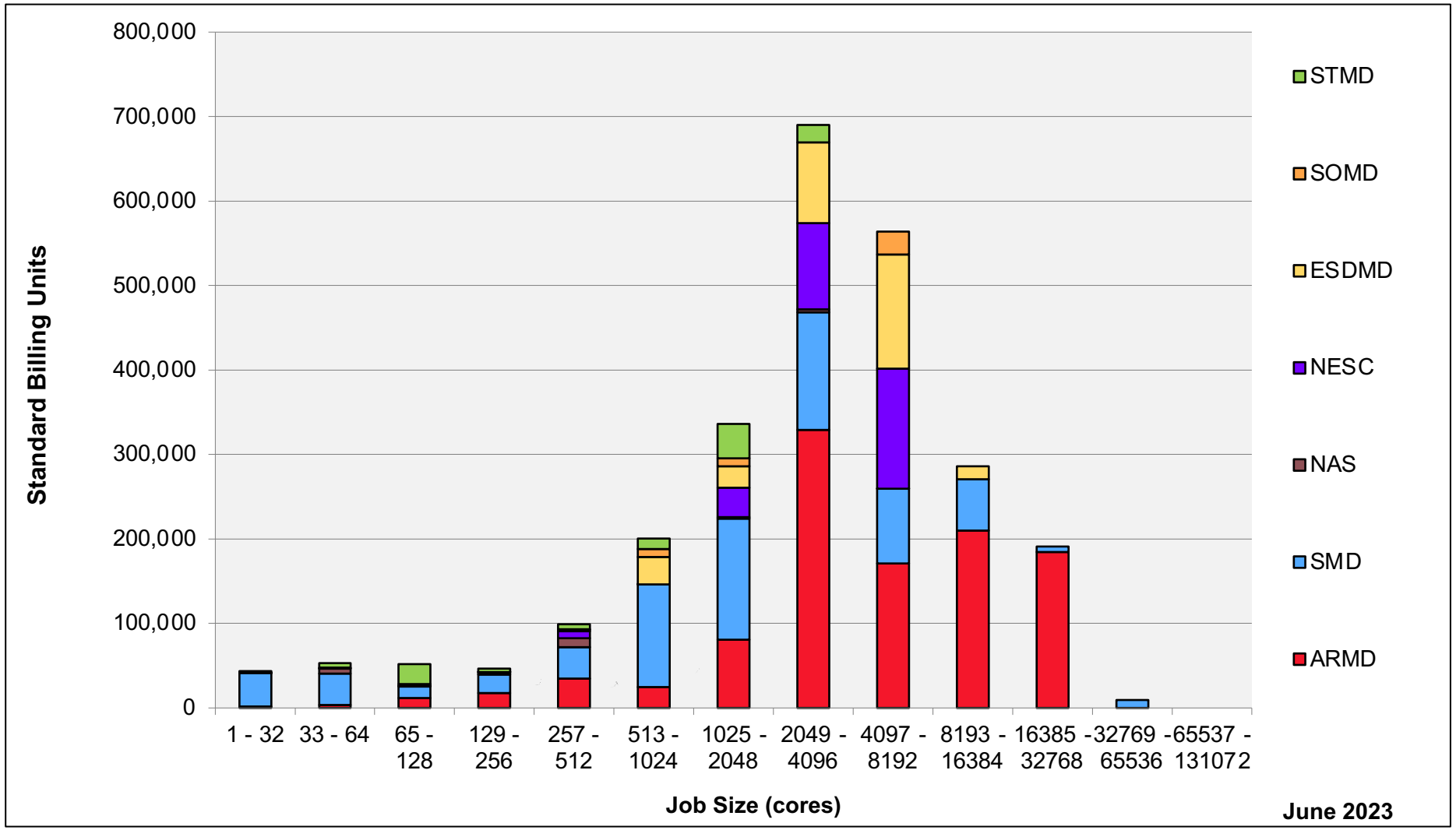
Electra: Devel Queue Utilization



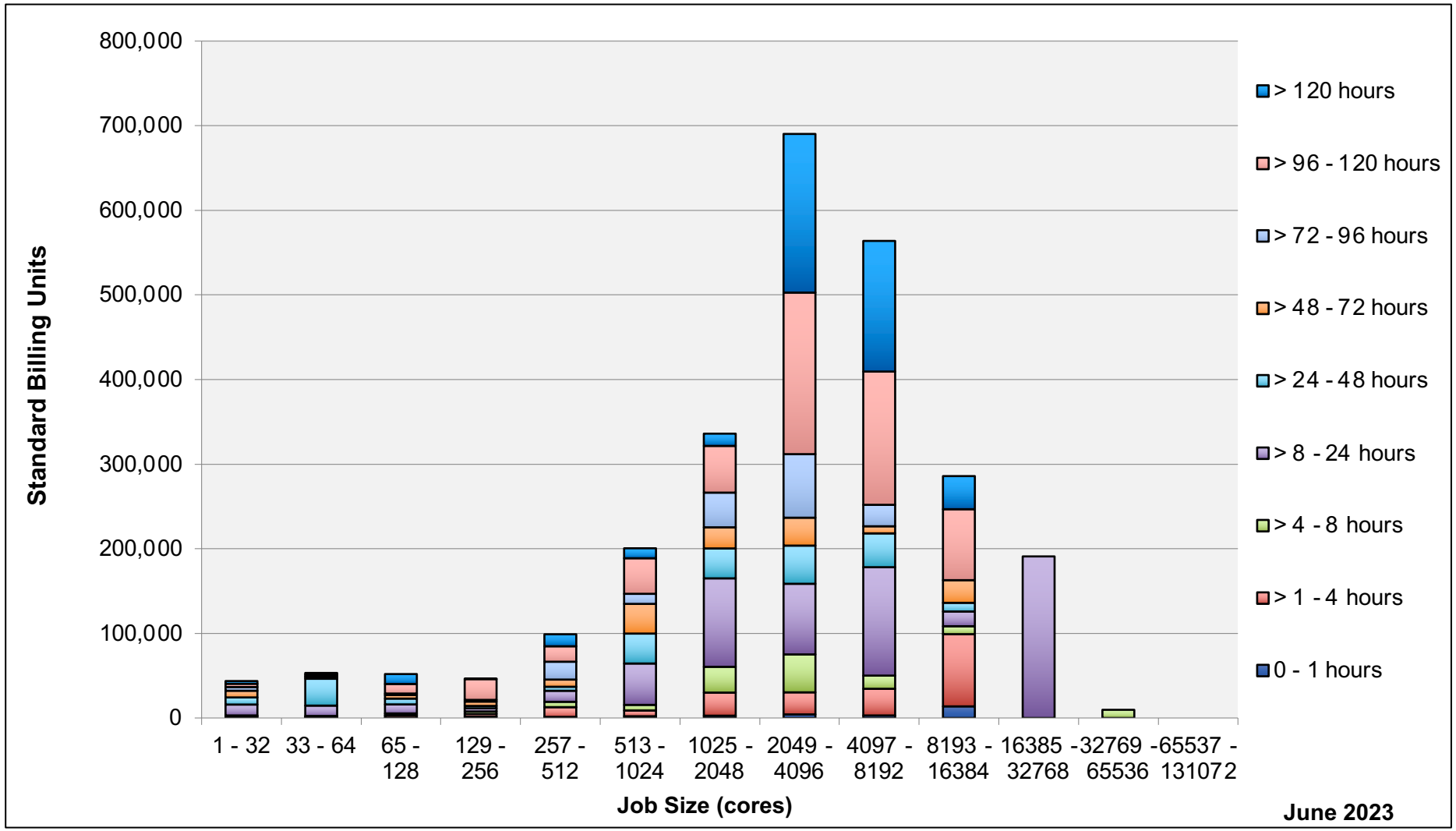
Electra: Monthly Utilization by Job Length



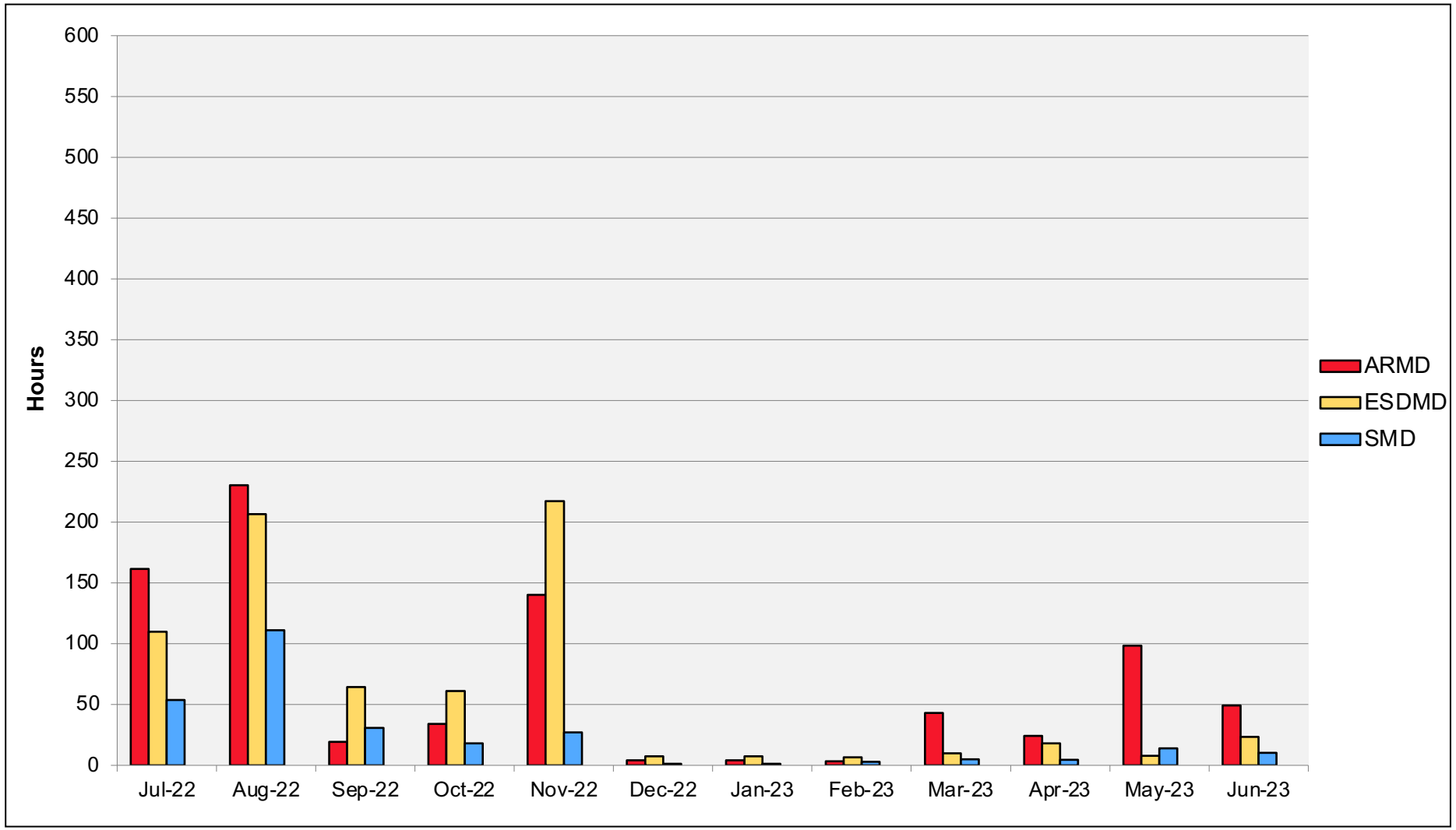
Electra: Monthly Utilization by Job Size



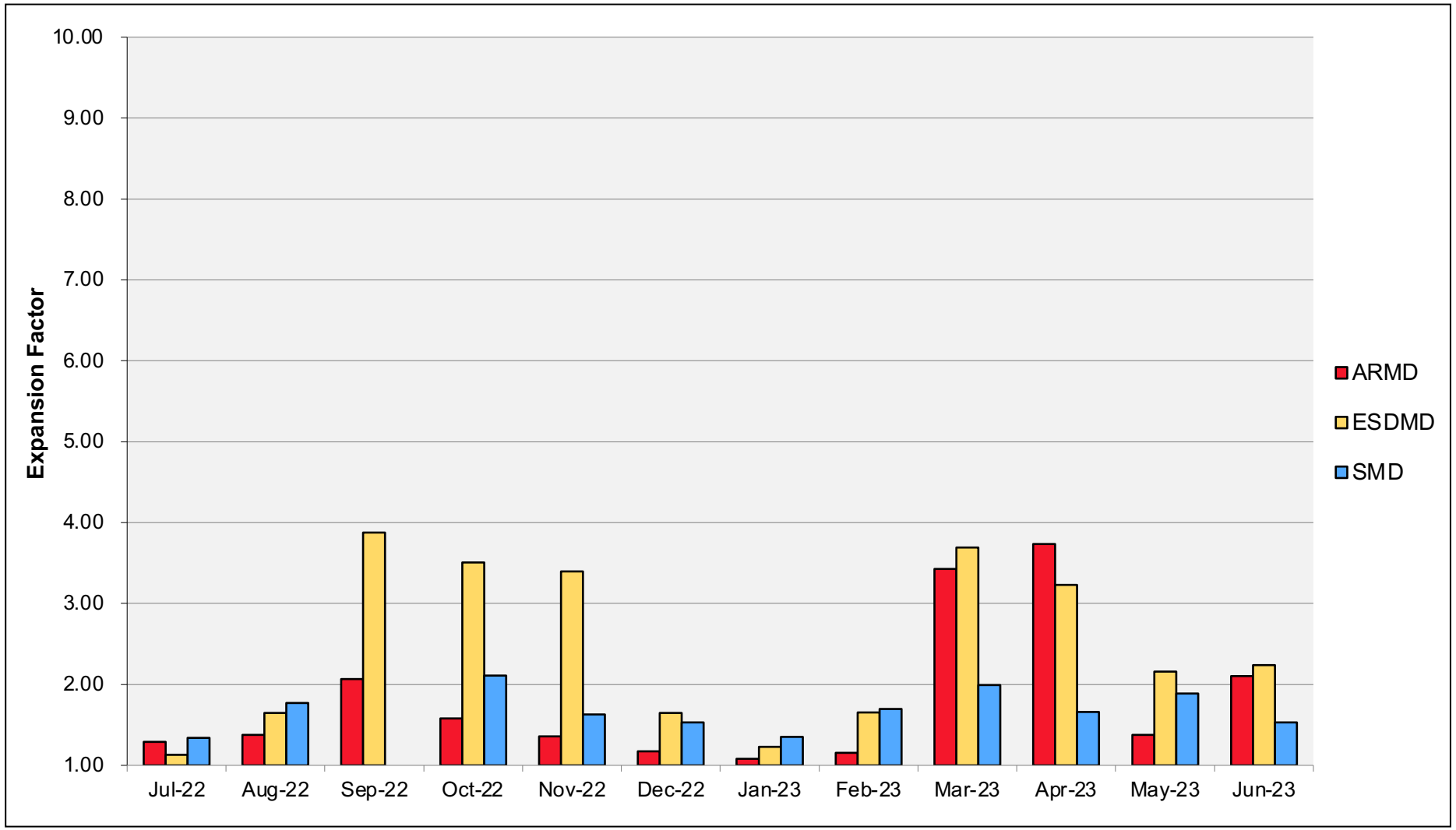
Electra: Monthly Utilization by Size and Length



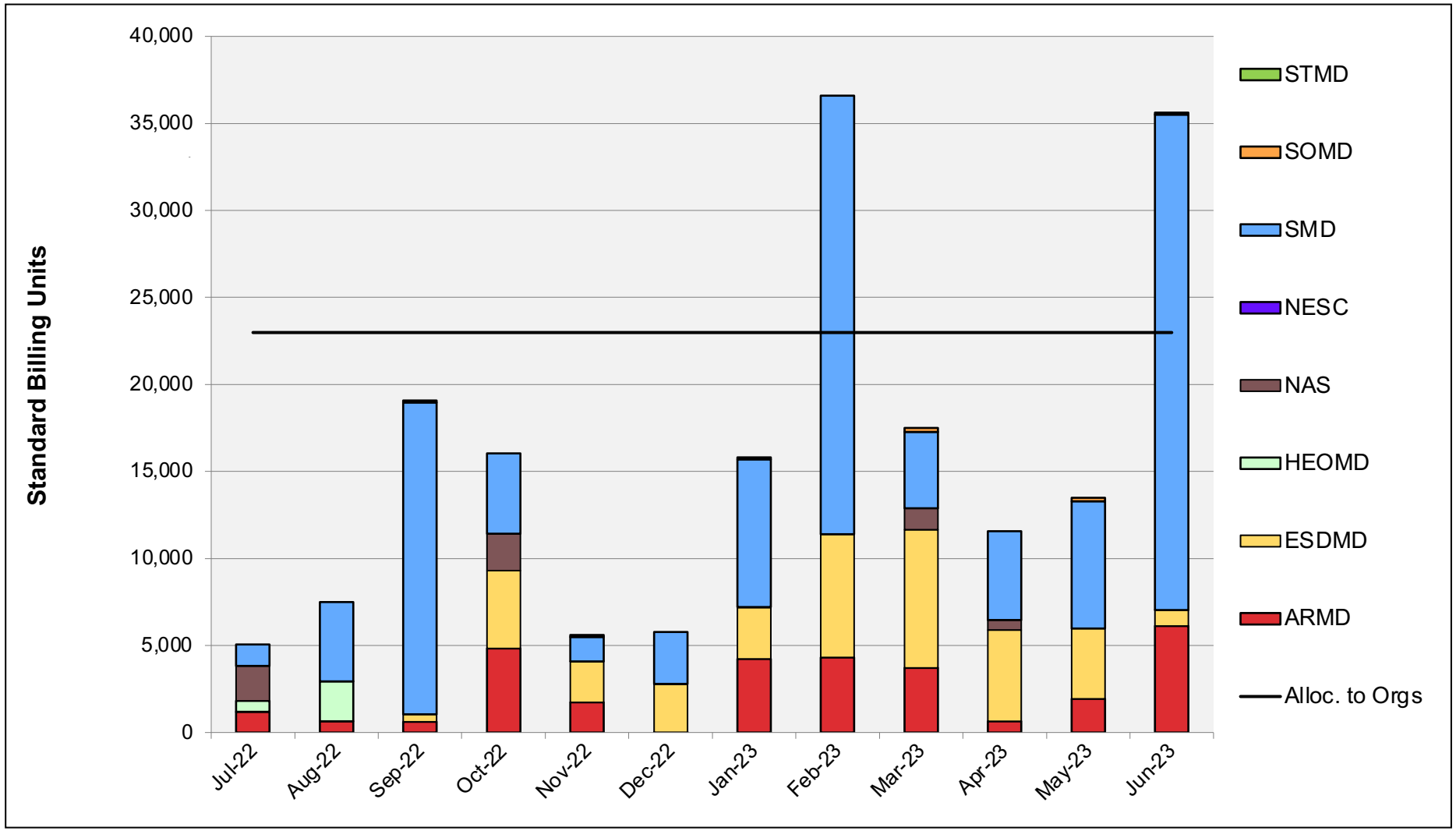
Electra: Average Time to Clear All Jobs



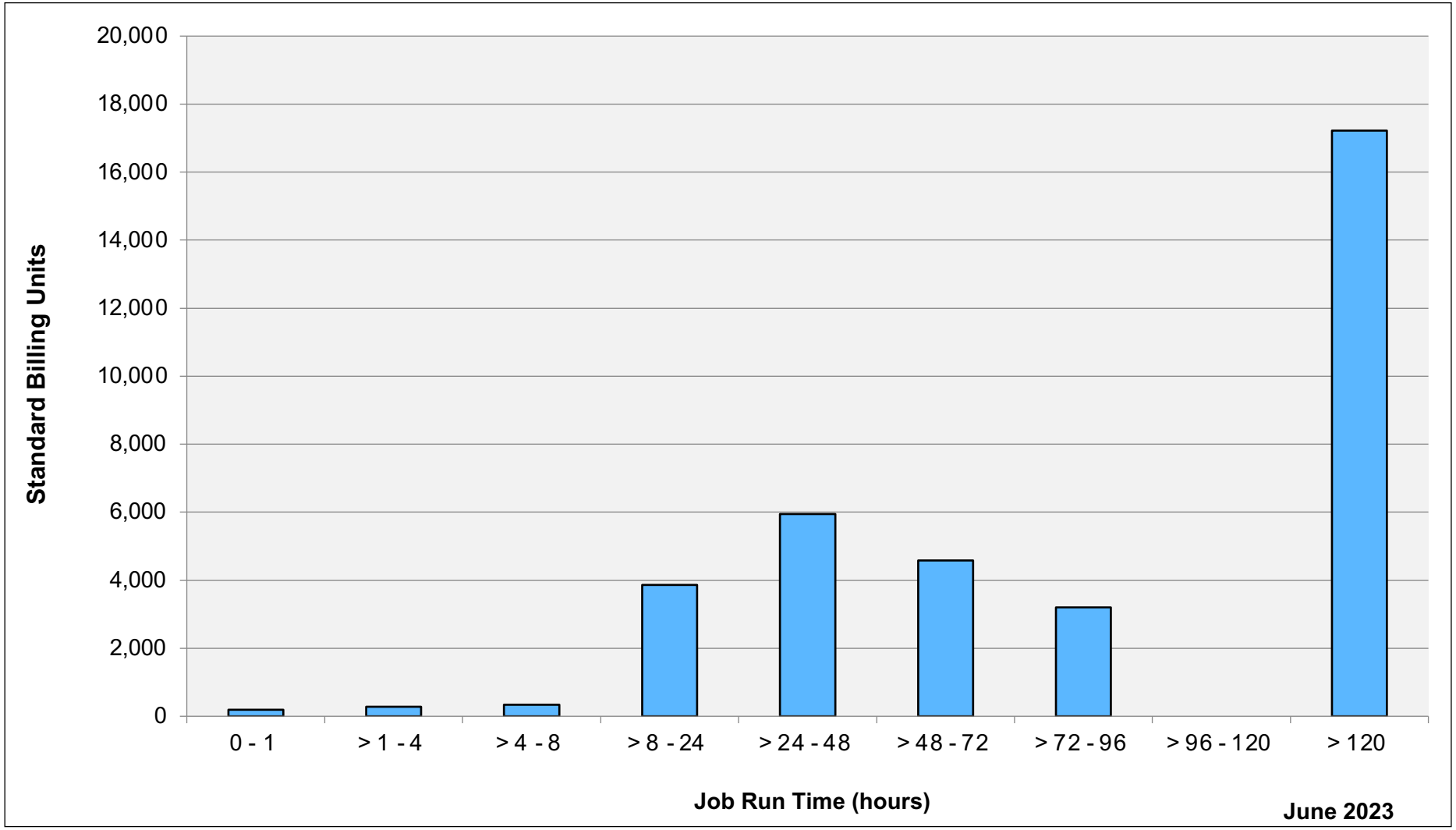
Electra: Average Expansion Factor



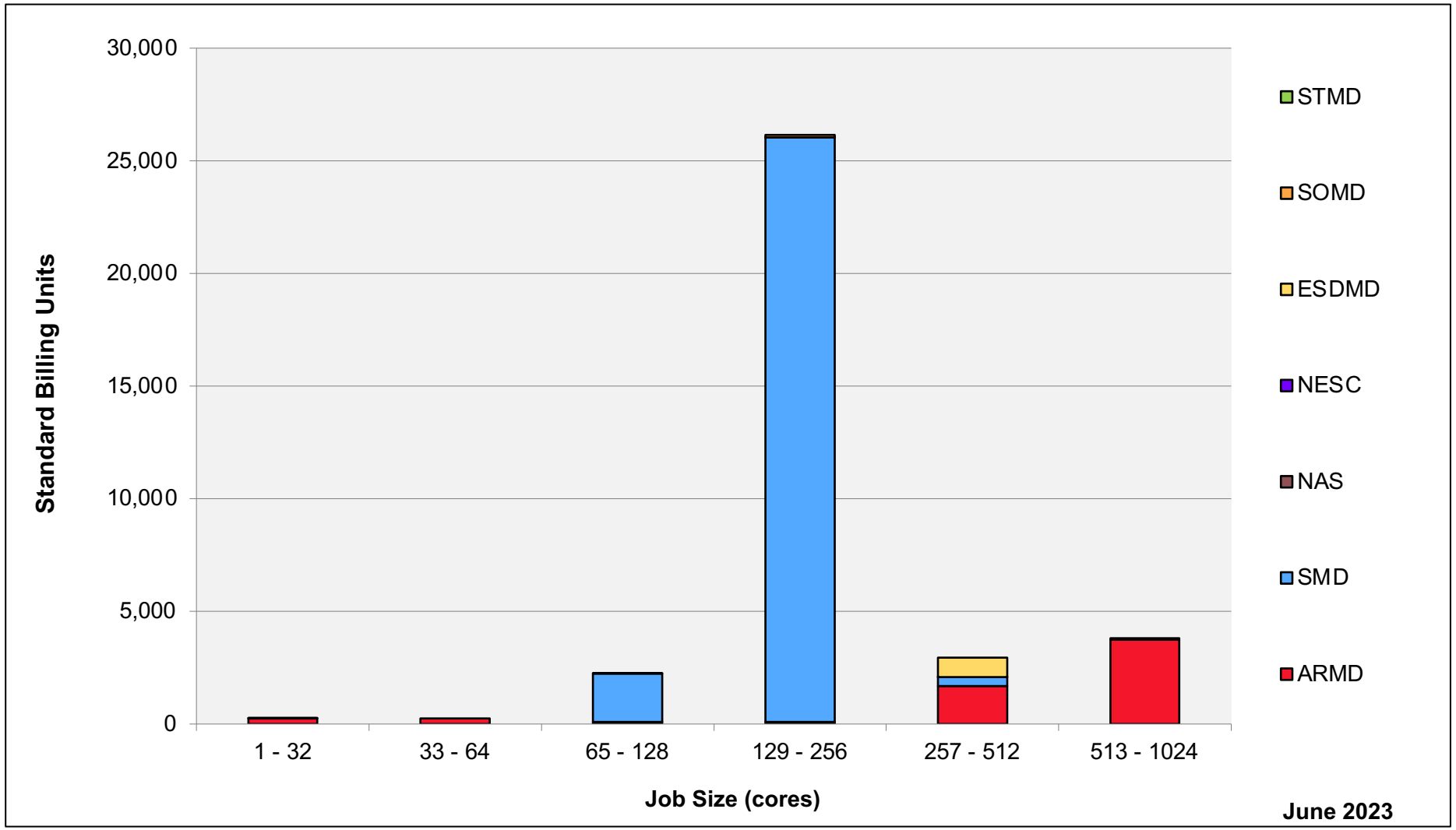
Endeavour: SBUs Reported, Normalized to 30-Day Month



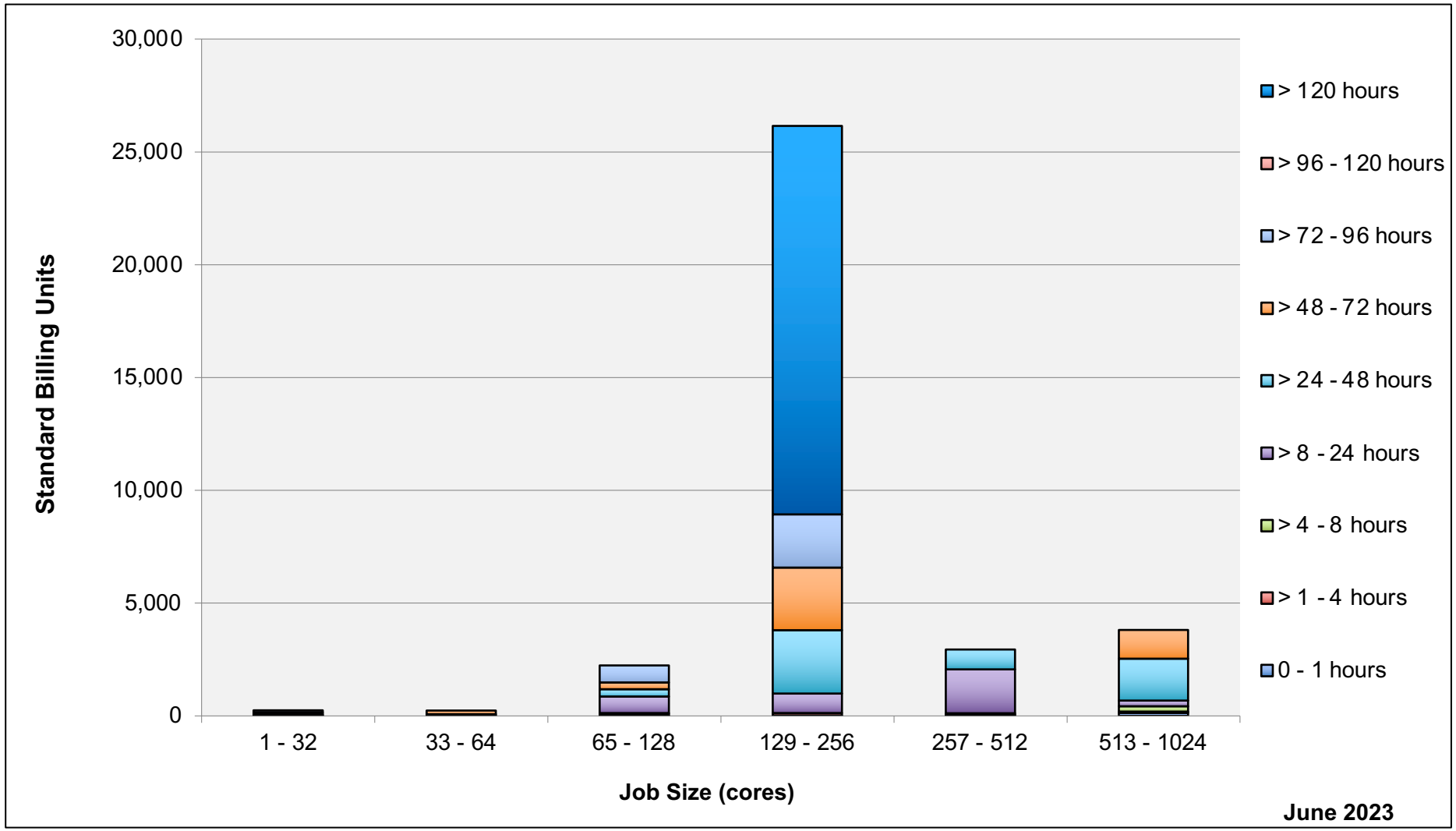
Endeavour: Monthly Utilization by Job Length



Endeavour: Monthly Utilization by Job Size



Endeavour: Monthly Utilization by Size and Length



Endeavour: Average Expansion Factor

