

National Aeronautics and Space Administration

HIGH-END COMPUTING CAPABILITY PORTFOLIO

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NASA Advanced Supercomputing Division

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HECC Completes Successful TOSS 4 and HPCM Migrations

- Due to NASA security requirements, HECC teams successfully transitioned most systems to the Red Hat Enterprise Linux 8-based Tri-Lab Operating System Stack Version 4 (TOSS 4).
- The extensive upgrade, which rolled out over five weeks, included all the Pleiades compute (CPU and GPU) and front-end nodes; the Aitken, Electra, and Endeavour nodes; the Lou mass storage system and its front ends; and the Portable Batch System servers.
- The biggest challenge of the migration from TOSS 3 to TOSS 4 for users was the move from Python 2 to Python 3. This required all users to update their software to use Python 3.
- Another impact for users is from the compatibility of user codes with new system libraries, including MPI libraries.
- The teams also replaced the old SGI-supported management software with the HPE Performance Cluster Manager (HPCM).
  - The primary challenge of migrating to HPCM was integration. The new HPCM software did not natively support HECC's older generation hardware and could not support Red Hat Enterprise Linux 8 (RHEL 8). HECC and HPE staff worked together to bridge the gap to make the new work with the old.
- HECC is leveraging interagency HPC work in operating systems and application scaling. Each organization continues to contribute improvements to the TOSS kernel.

IMPACT: Migrating to the TOSS4 provides an upgraded software environment using Python 3 and enhanced security.

Lawrence Livermore National Laboratory

Los Alamos NATIONAL LABORATORY EST. 1943

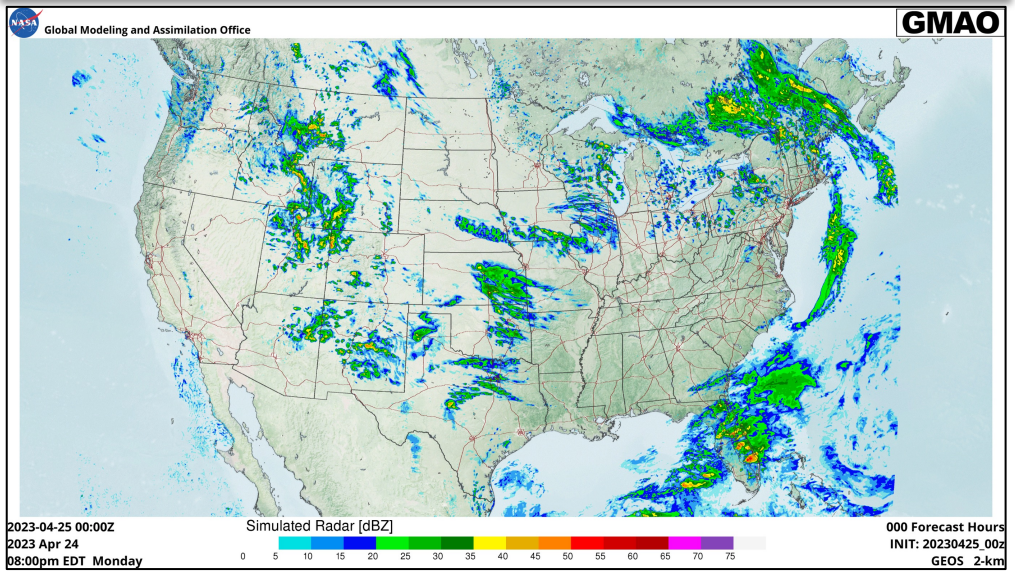
Sandia National Laboratories

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.

APP Concierge Service Supports Spring Weather Forecast

- HECC Applications Performance and Productivity (APP) experts are providing customized debugging and job execution assistance to the Goddard Spring Forecast Experiment on daily and nightly advance reservations over a continuous 10-week period (March 30 through about mid-June, 2023).
- APP staff adjusted nightly reservations of 420 AMD Rome nodes to daytime hours when assistance from Goddard Earth Observing System (GEOS) code developers was needed; and monitored job progress in the nightly runs and adjusted reservation end times to ensure completion of all jobs.
  - The team extensively investigated the reasons jobs in the reservation would not start running and documented the causes and fixes for each one. If a job failed due to a bad node or hung in the middle of a run, APP off-lined the bad node(s) and resubmitted the job to be rerun.
- APP worked with Control Room analysts (CRAs) to document the job monitoring task, including troubleshooting why jobs won't start, collecting stack traces when jobs hang, and extending the reservation time as needed. These troubleshooting tips and tricks will be useful for CRAs responding to future problem reports related to getting jobs started in reservations.

IMPACT: The extensive and continuous expert assistance from HECC applications experts enabled successful GMAO nightly runs of the Spring Hazardous Weather Forecasts. The work included training of Control Room analysts to augment their skill set and assist with taking corrective actions.

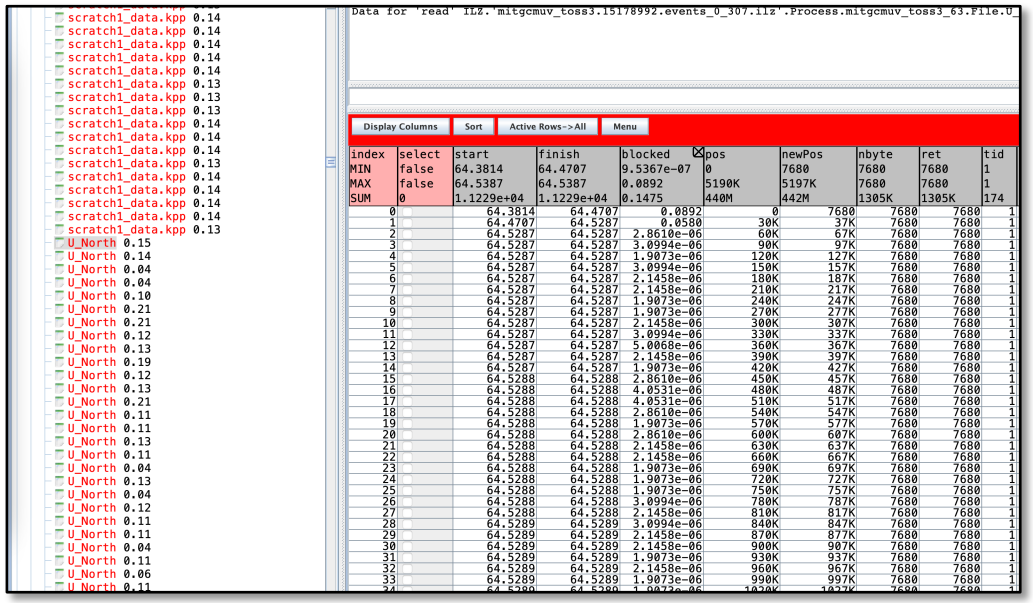


The Spring Hazardous Forecast Experiment is a comprehensive evaluation of multiple contributing models, including the GEOS model, with a focus on severe weather over the continental U.S., representation of simulated reflectivity, updraft, and rotation properties, and environmental variables. *William Putman/GSFC*

APP Team Assembles I/O Benchmarking Suite

- HECC's Application Performance and Productivity (APP) team recently completed the testing, characterization, and collection of four I/O-intensive applications for examining new or regression-testing existing I/O systems.
- A benchmarking suite was created in response to the need for standardizing the I/O testing and comparing in a way similar to the HECC Standard Billing Units (SBU-1 and SBU-2) benchmarks, which focus on CPU, cache, memory, and communication performance but had lacked the I/O component.
- The suite is stored in an APP repository on Pleiades for easy access and testing by HECC support staff. It includes:
  - Four applications: NAS Parallel Benchmark Block-Tridiagonal IO (BTIO), HDF5 Group's H5Perf, NAS in-house Astrophysics application StellarBox, and the MIT General Circulation Model (MITgcm) with in-house developed highly parallel input/output routines.
  - Description of each application's I/O characteristics uncovered via I/O profiling tools such as MPIProf, Darshan, and IOT.
  - Build and run instructions, sample job scripts, and sample output files for comparison.
- The APP team will continue to expand the suite when other suitable applications are encountered.

IMPACT: The availability of an I/O benchmark suite with documentation in a centralized repository allows for knowledge sharing and retention. In addition, the suite enables any member of the HECC technical team to perform I/O testing.

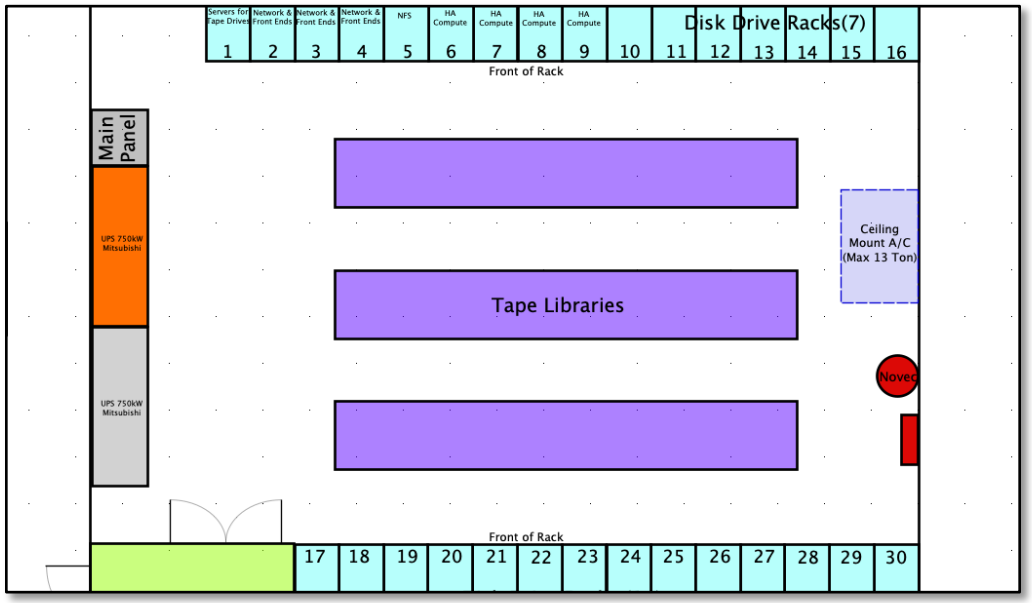


Screenshot showing the characterization of the MITgcm model I/O via the IOT tool. This table shows the time line (start, finish, blocked), file position (position, newposition after read), and size (nbyte read and bytes returned) of one MPI rank reading one of the input files (U North).

Data Module Request for Information Released to Vendors

- A Request for Information (RFI) for a new data module to be located near the existing Aitken module at the Modular Supercomputing Facility (MSF) was released to potential vendors on May 3, 2023.
  - The RFI's purpose is to identify capable vendors to design and manufacture a modular data center focused on housing data storage equipment.
  - The RFI requests vendors to provide input to the Data Module Requirements Document to improve the document prior to release in the Request for Proposal (RFP).
  - Vendor RFI responses are due June 8, 2023, with the goal to release the RFP to bidders on June 29, 2023 and module use in early 2025.
- The data module will house data storage equipment at the MSF, providing a fully capable, standalone data center.
  - Currently, the MSF only houses the Aitken supercomputer—all HECC filesystems are housed in either the main NAS facility (building N258), or a secondary facility (building N233A).
- The module will house the redundant tape libraries, new hard-disk and solid-state storage drives, routers, front ends, network, and high-availability compute; and will feature an Uninterruptible Power Supply with generator backup during power outages.

IMPACT: A new data module at the Modular Supercomputing Facility will locate data storage near the Aitken supercomputer, improving performance and providing additional storage resources for HECC users.



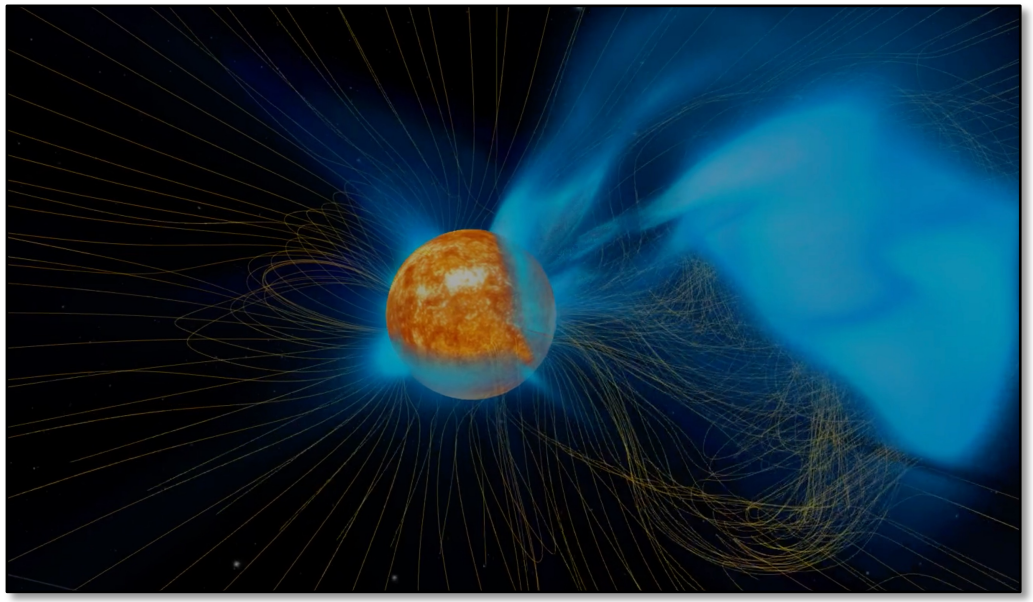
Conceptual layout of the new data module to be located at the Modular Supercomputing Facility at NASA's Ames Research Center. *Chris Tanner, NASA/Ames*

Simulating Solar Storms for Space Weather Prediction*

- Computational scientists at Predictive Science Inc. developed the CORona-HELiosphere Automated Multiple CME Generator (CORHEL-AMCG) framework to successfully model real solar storm events involving multiple eruptions, including coronal mass ejections (CMEs).
  - Mechanisms that control CME properties are poorly understood and challenging to model empirically.
  - This new framework allows non-expert users to routinely model multiple CMEs in a realistic coronal and solar-wind environment and propagate them to Earth.
- These simulations require grids of up to 50 million cells and integration of time-dependent equations for millions of cycles. They require around 20 hours on 32 Electra nodes to complete.
- The solar storm event simulations are used to model and study solar energetic particle events, which can pose a danger to astronauts in interplanetary space.
- The CORHEL-AMCG framework is being integrated into a public run-on-demand system at CCMC, allowing researchers to generate solar storm simulations from the Sun to Earth, a key tool for improving space weather prediction.

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

IMPACT: Coronal mass ejections can disrupt radio transmissions, damage satellites, and severely impact power transmission grids. Modeling such eruptions and their properties is of great importance and a major goal of NASA's Heliophysics Research Program.

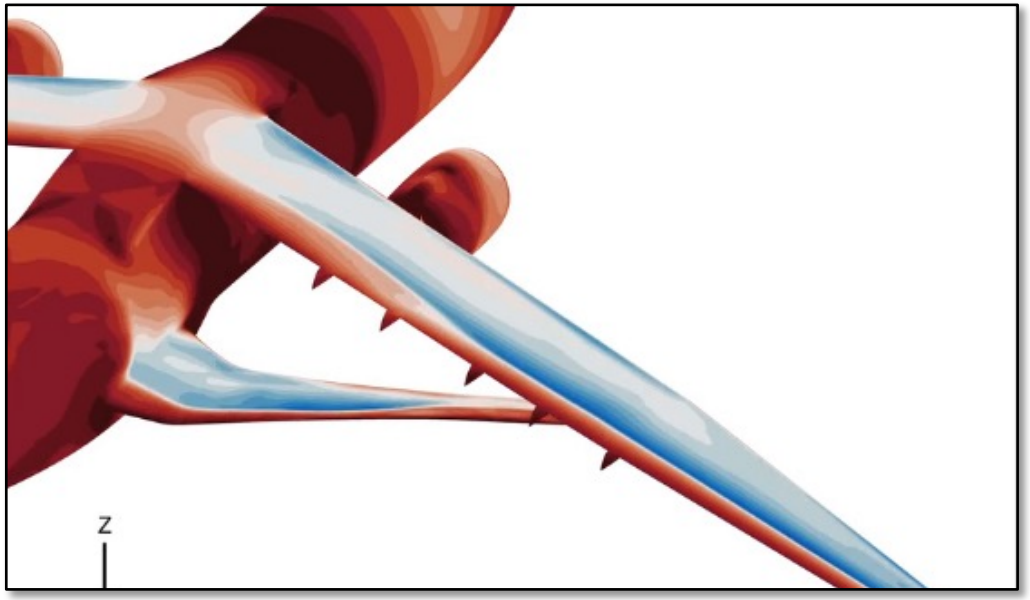


Snapshot from a simulation of the solar storm that occurred on July 14, 2000, using the magnetohydrodynamics code (MAS) utilized in CORHEL-AMCG. The density and magnetic field lines are shown near the start of the eruption. The visualization shown is using the OpenSpace interactive software. *Tibor Török, Predictive Science Inc.*

High Fidelity Hybrid Electric TTBW Simulation Capability*

- The unconventional configuration of the Transonic Truss-Braced Wing (TTBW) concept design leads to complex flow phenomena that are challenging to simulate—such as transonic buffet, separated flow, and a turbulent wake.
- Using the Aitken supercomputer, NASA Ames researchers ran Unsteady Reynolds Averaged Navier-Stokes (URANS) simulations and Hybrid RANS Large Eddy Simulations (HRLES) to evaluate the accuracy and efficiency of both approaches to simulating the TTBW.
- Results indicate that URANS may perform better than HRLES in predicting buffet onset at a lower computational cost; however, its accuracy tends to decrease for certain conditions, and scale-resolving methods are necessary to conduct further vehicle analysis. The TTBW design incorporates advancements in technology that may improve fuel efficiency for commercial aircraft.
- Overall, the team gained a deeper understanding about the TTBW concept and shared those findings with the TTBW project and other NASA teams. This work will reduce future cost by improving HRLES simulations and determining the levels of uncertainty for all. methods

IMPACT: In the pursuit of a more fuel-efficient narrowbody commercial aircraft design, NASA invests a considerable resources toward research into transonic truss-braced wing (TTBW) concepts. By improving understanding of this type of aircraft, the Ames work will help the Agency develop a flight demonstrator.



Simulation of instantaneous surface pressure coefficient contour (red is high, blue is low) for the TTBW concept aircraft in the free-air configuration from a freestream initial condition. *Oliver Browne, NASA/Ames*

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Papers

- "**Magnetotail Ion Acceleration in 3D Global Hybrid Simulations**," F. Shi, Z. Guo, Y. Lin, X. Wang, L. Cheng**,** Journal of Geophysical Research: Space Physics, May 1, 2023. *
  https://agupubs.onlinelibrary.wiley.com/doi/full/10.1029/2022JA030980
- "**Multiplicity Boost of Transit Signal Classifiers: Validation of 69 Exoplanets Using the Multiplicity Boost of ExoMiner**," H. Valizadegan, et al., arXiv:2305.02470 [astro-ph.EP], May 4, 2023. *
  https://arxiv.org/abs/2305.02470
- "**Multi-Oligomeric States of Alamethicin Ion Channel: Assemblies and Conductance**," C. Wei, A. Pohorille, Biophysical Journal, May 8, 2023. *
  https://www.cell.com/biophysj/pdf/S0006-3495(23)00304-1.pdf
- "**An Unusually Low-Density Super-Earth Transiting the Bright Early-Type M-Dwarf GJ 1018 (TOI-244)**," A. Castro-González, et al., arXiv:2305.04922 [astro-ph.EP], May 8, 2023. *
  https://arxiv.org/abs/2305.04922
- "**Efficient Quasi-Classical Trajectory Calculations by Means of Neural Operator Architectures**," M. Priyadarshini, et al., Physical Chemistry Chemical Physics (Royal Society of Chemistry), May 9, 2023. *
  https://pubs.rsc.org/en/content/articlehtml/2023/cp/d2cp05506f
- "**Modeling the Recent Changes of Phytoplankton Blooms Dynamics in the Arctic Ocean**," M. Manizza, et al., Journal of Geophysical Research: Oceans, published online May 9, 2023. *
  https://agupubs.onlinelibrary.wiley.com/doi/abs/10.1029/2022JC019152

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

Papers (cont.)

- "**Dust Impacts on Mongolian Cyclone and Cold Front in East Asia: A Case Study During 18-22 March 2010**," J. Li, S.-H. Chen, Frontiers Environmental Science (Atmosphere and Climate), May 19, 2023. *
  https://www.frontiersin.org/articles/10.3389/fenvs.2023.1167232/full
- "**Molecular Dynamics Simulation of Twin Nucleation and Growth in Ni-Based Superalloys**," V. Borovikov, et al., International Journal of Plasticity, vol. 166, published online May 15, 2023. *
  https://www.sciencedirect.com/science/article/abs/pii/S0749641923001316
- "**TOI-2498 b: A Hot Bloated Super-Neptune within the Neptune Desert**," G. Frame, et al., Monthly Notices of the Royal Astronomical Society, vol. 523, issue 1, published online May 16, 2023. *
  https://academic.oup.com/mnras/article/523/1/1163/7165762
- "**Satellite Remote-Sensing Capability to Assess Tropospheric-Column Ratios of Formaldehyde and Nitrogen Dioxide: Case Study During the Long Island Tropospheric Ozone Study 2018 (LISTOS 2018) Field Campaign**," M. Johnson, et al., Atmospheric Measurement Techniques, published May 16, 2023. *
  https://amt.copernicus.org/articles/16/2431/2023/amt-16-2431-2023.pdf
- "**A Temperate Earth-Sized Planet with Tidal Heating Transiting an M6 Star**," M. Peterson, et al., Nature, vol. 617, May 17, 2023. *
  https://www.nature.com/articles/s41586-023-05934-8
- "**A 1.55 $R_{\oplus}$ Habitable-Zone Planet Hosted by TOI-715, and M4 Star Near the Ecliptic South Pole**," G. Dransfield, et al., Monthly Notices of the Royal Astronomical Society, published online May 18, 2013. *
  https://academic.oup.com/mnras/advance-article/doi/10.1093/mnras/stad1439/7172075

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Papers (cont.)

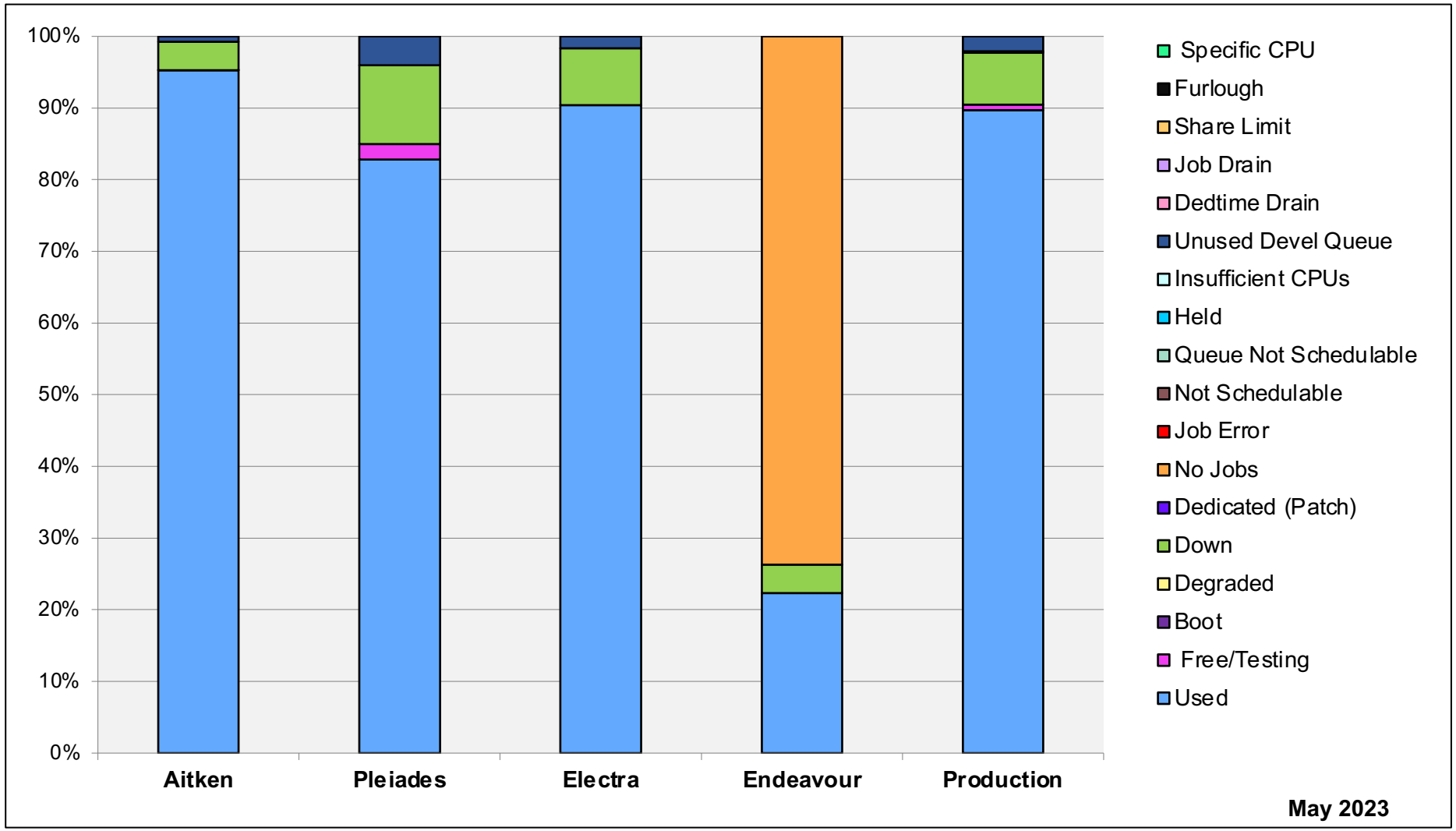
- "**Anisotropic Satellite Galaxy Quenching: A Unique Signature of Energetic Feedback by Supermassive Black Holes?**" J. Karp, et al., The Astrophysical Journal Letters, vol. 949, no. 1, May 23, 2023. *
  https://iopscience.iop.org/article/10.3847/2041-8213/acd3e9
- "**TOI-1859b: A 64-Day Warm Jupiter on an Eccentric and Misaligned Orbit**," J. Dong, et al., arXiv:2305.16495 [astro-ph.EP], May 25, 2023. *
  https://arxiv.org/abs/2305.16495
- "**Modeling Carbon Nanotube Entanglement Load Transfer: Implications for Lightweight Aerospace Structures**," B. Jensen, et al., Applied Nano Materials (American Chemical Society), published online May 26, 2023. *
  https://pubs.acs.org/doi/abs/10.1021/acsanm.3c01255
- "**TOI-1416: A System with a Super-Earth Planet with a 1.07d Period**," H. Deeg, et al., arXiv:2305.18542 [astro-ph.EP], May 29, 2023. *
  https://arxiv.org/abs/2305.18542

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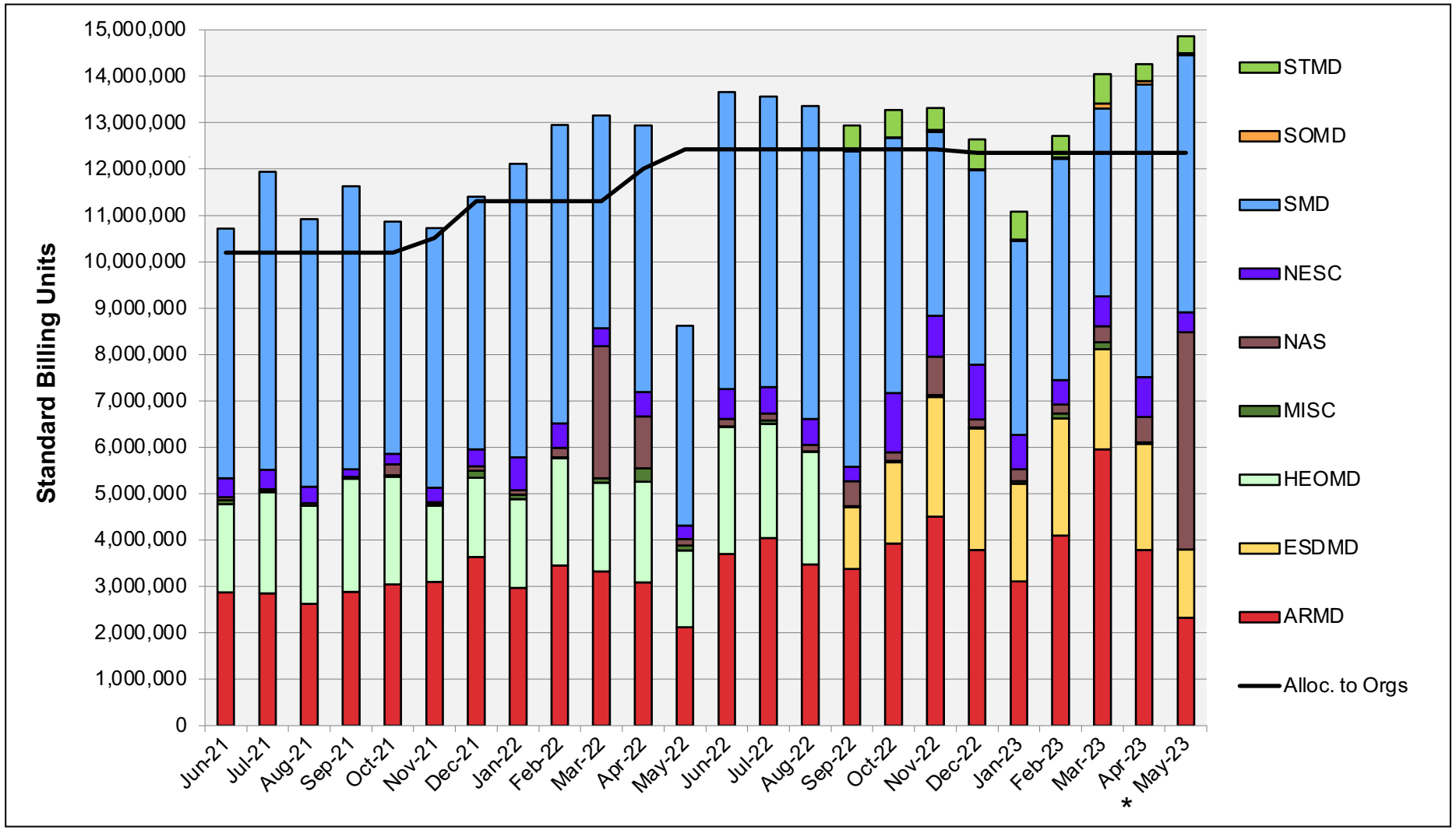
News and Events: Social Media

- **Coverage of NAS Stories**
  - History Guy feature on supercomputer at NASA Ames Research Center:
    - NASA Supercomputing: Facebook 21 reactions, 11 shares.
    - NAS Division: Twitter 6 retweets, 8 likes, ~1.2k views.
  - TESS Exoplanet Discovery:
    - NASA Exoplanets: Facebook 374 reactions, 110 shares; Twitter 138 retweets, 703 likes, ~118.1k views.
    - NASA Supercomputing: Facebook 21 reactions, 3 shares.
    - NAS Division: Twitter 25 retweets, 120 likes, ~42.8k views.

HECC Utilization

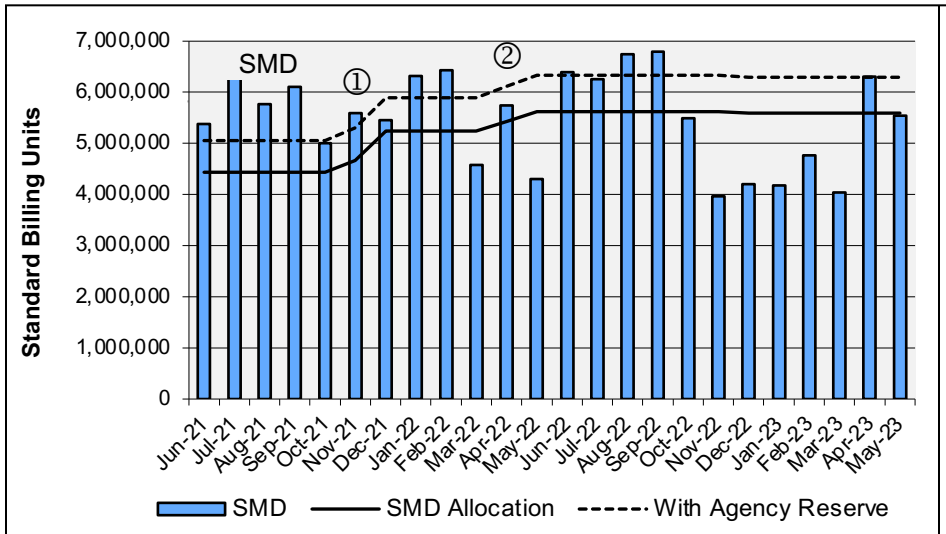


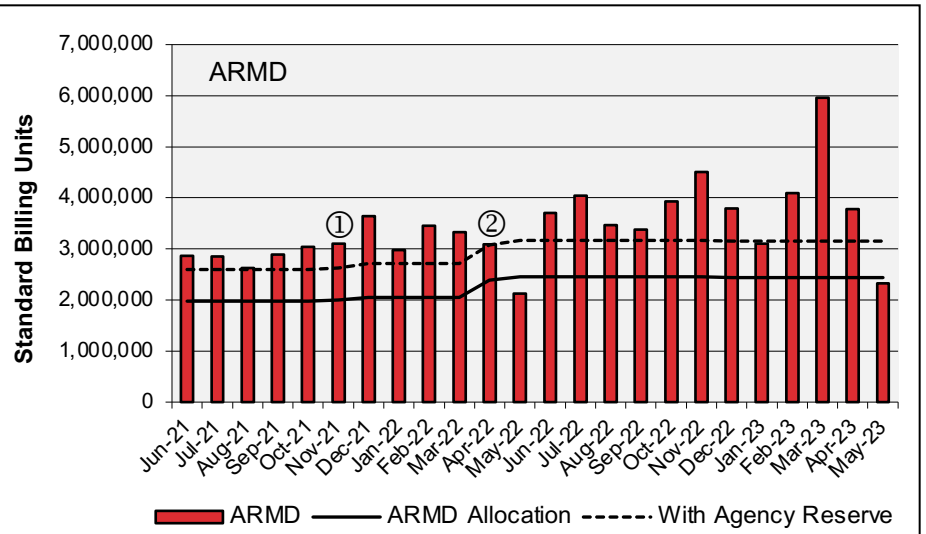
HECC Utilization Normalized to 30-Day Month

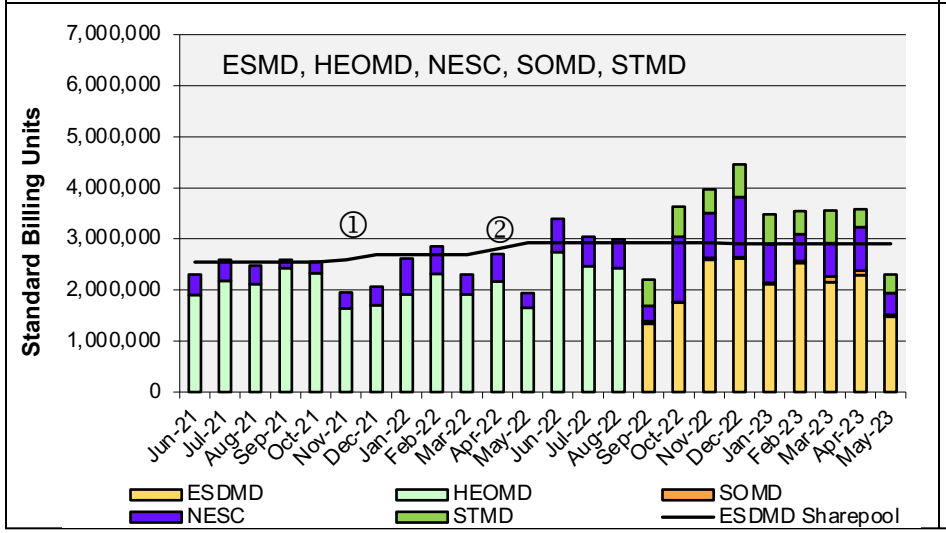


* The large NAS utilization was due to upgrading TOSS3 to TOSS4

HECC Utilization Normalized to 30-Day Month



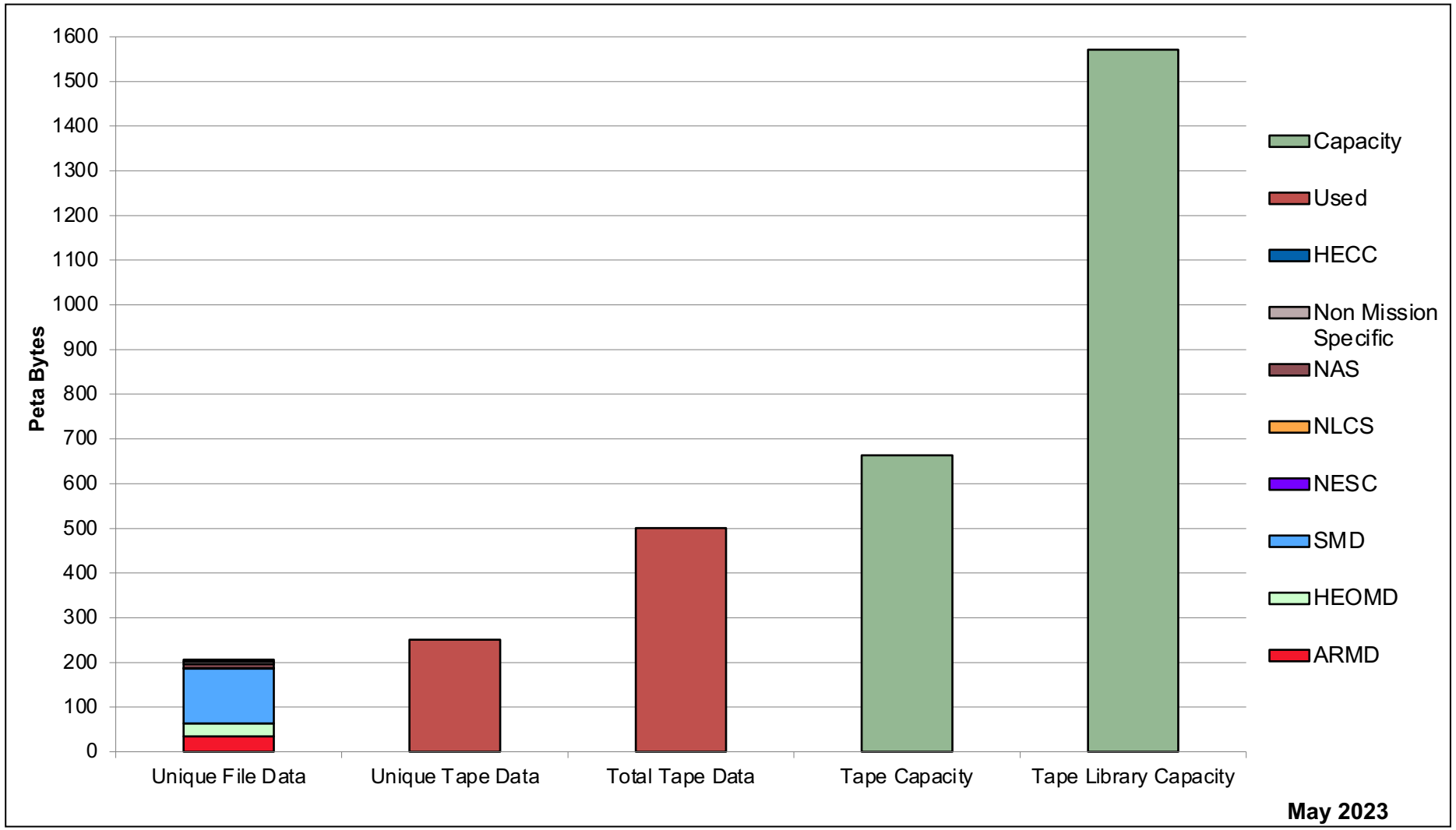




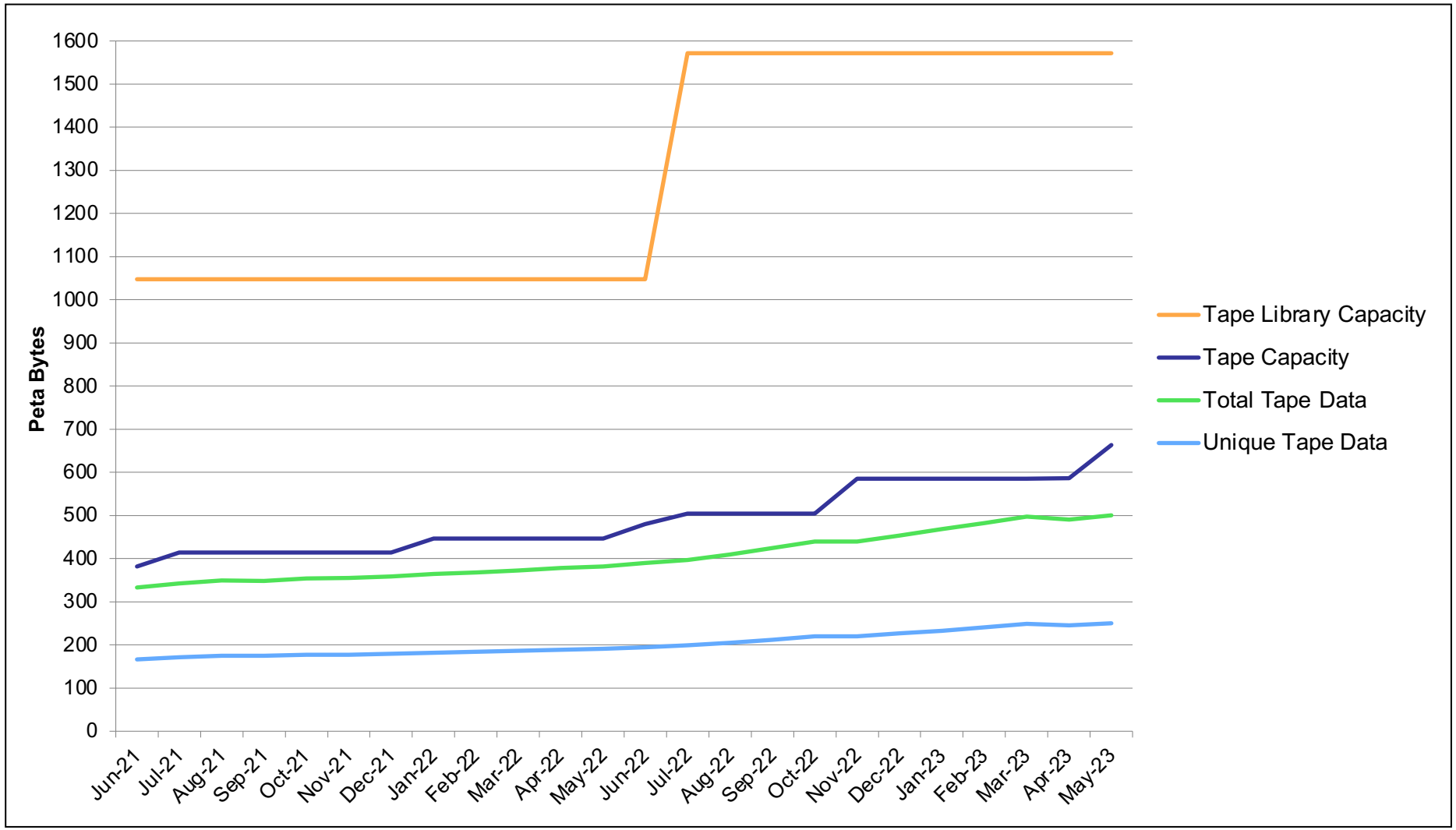
① 4 Rome Apollo Racks added to Aitken

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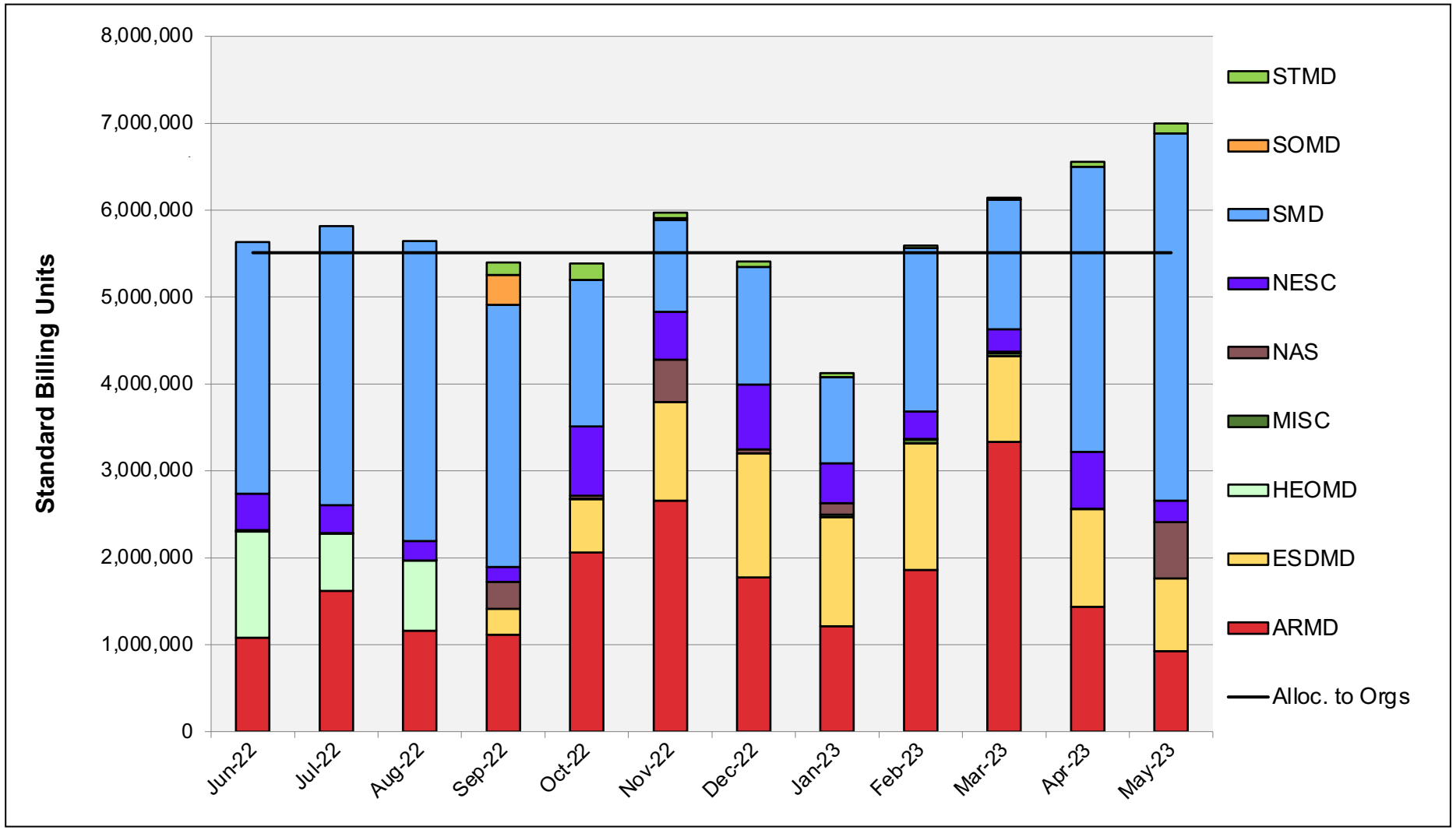
Tape Archive Status



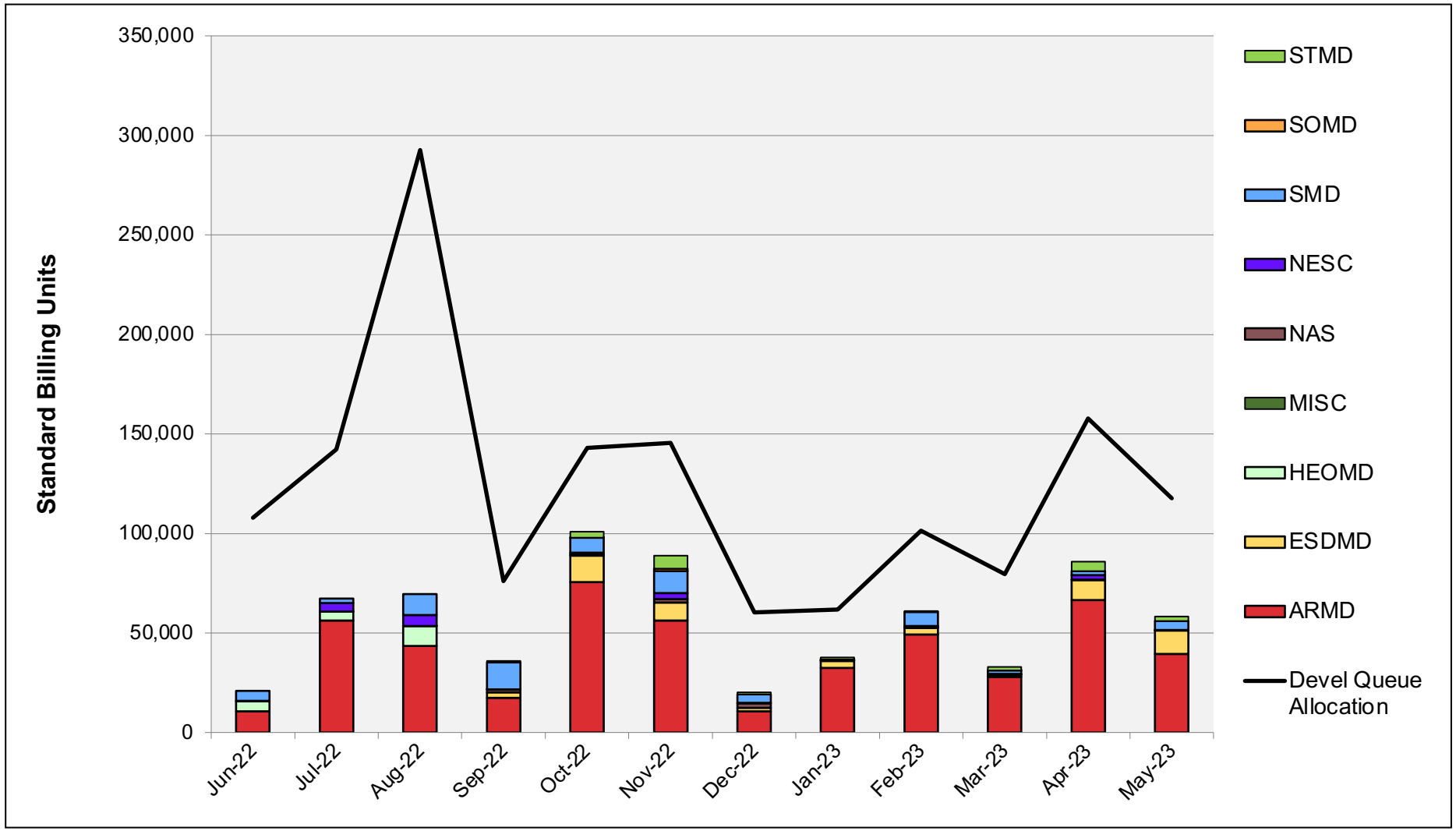
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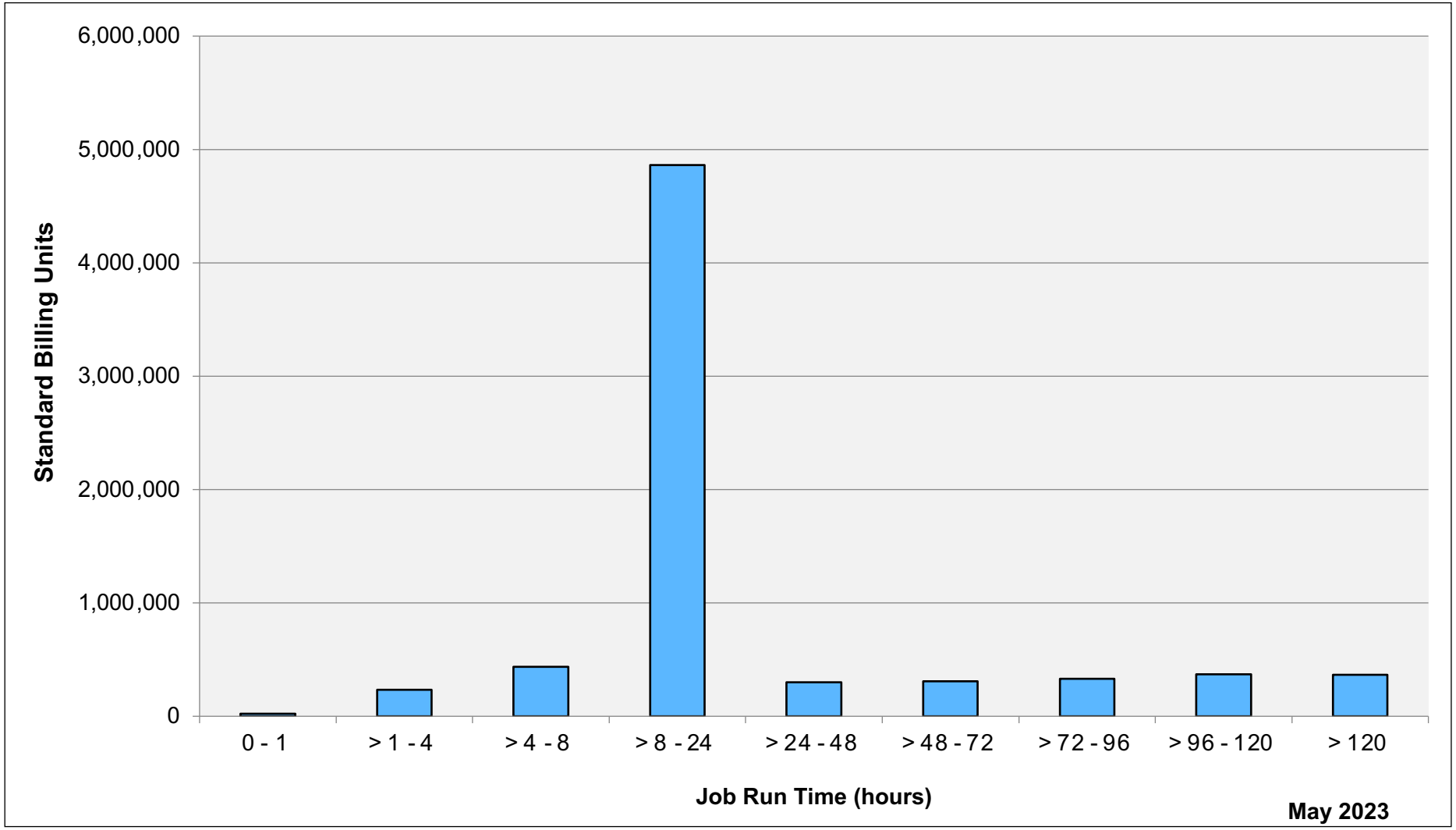
Aitken: SBUs Reported, Normalized to 30-Day Month



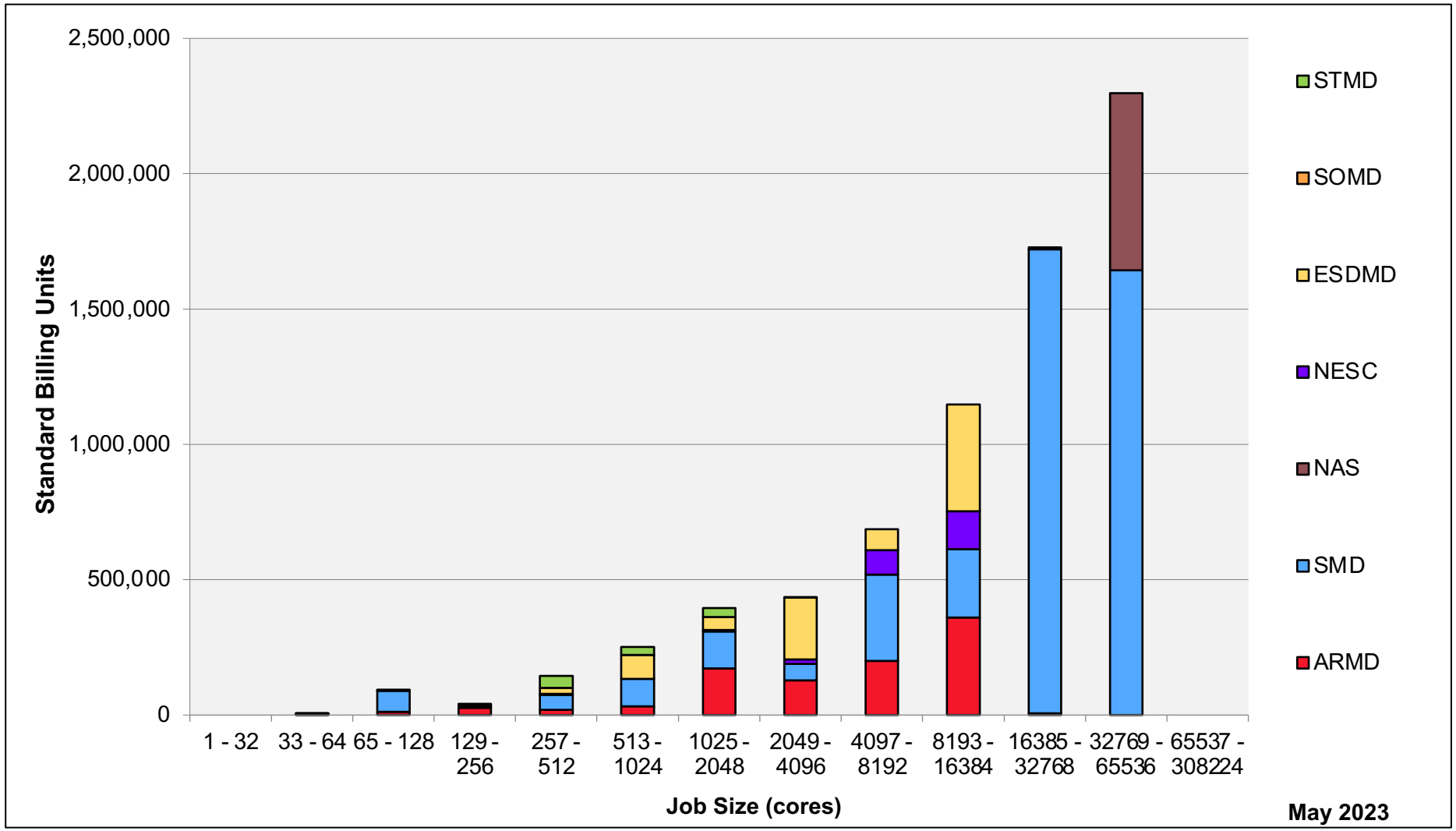
Aitken: Devel Queue Utilization



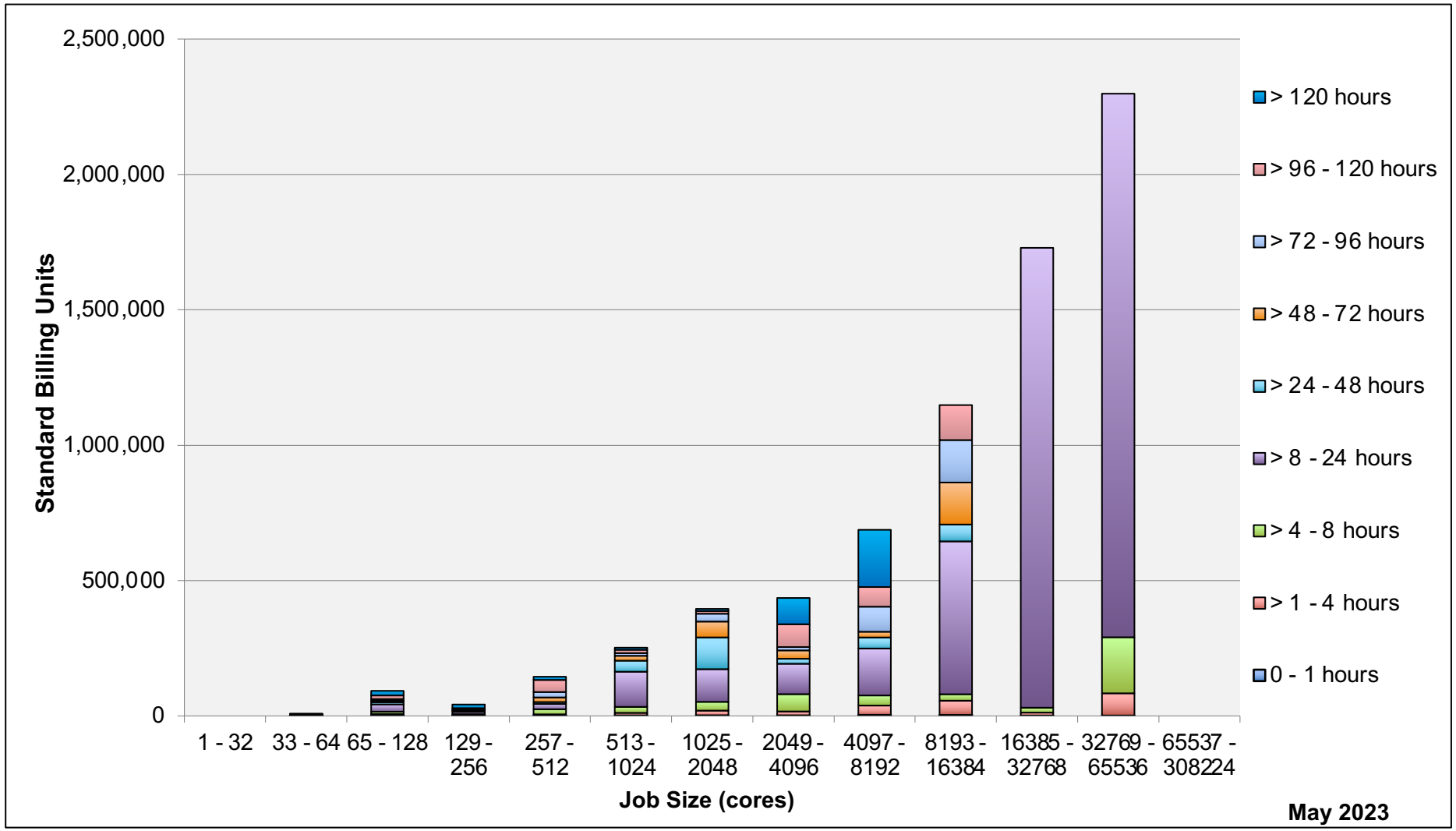
Aitken: Monthly Utilization by Job Length



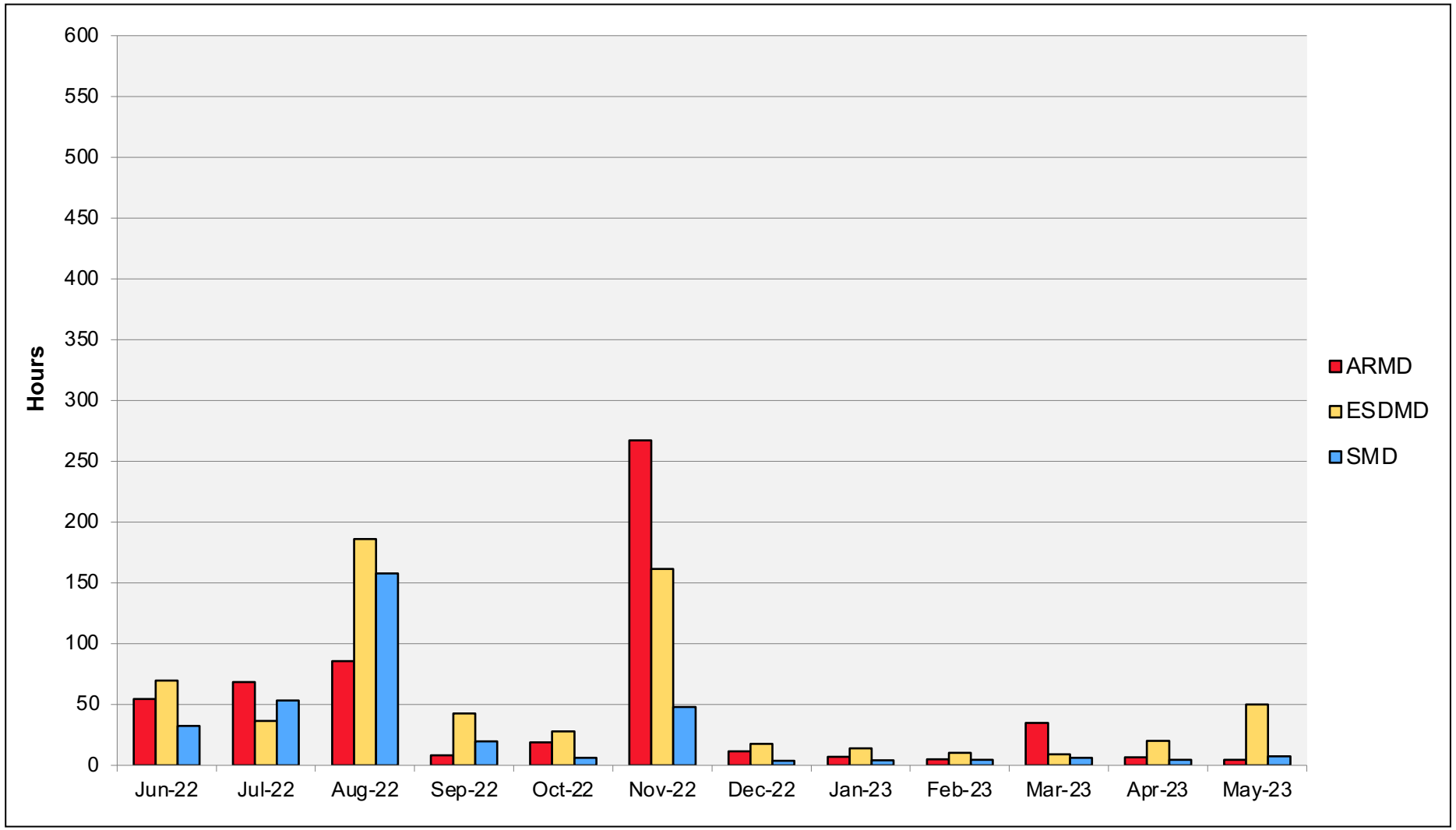
Aitken: Monthly Utilization by Job Size



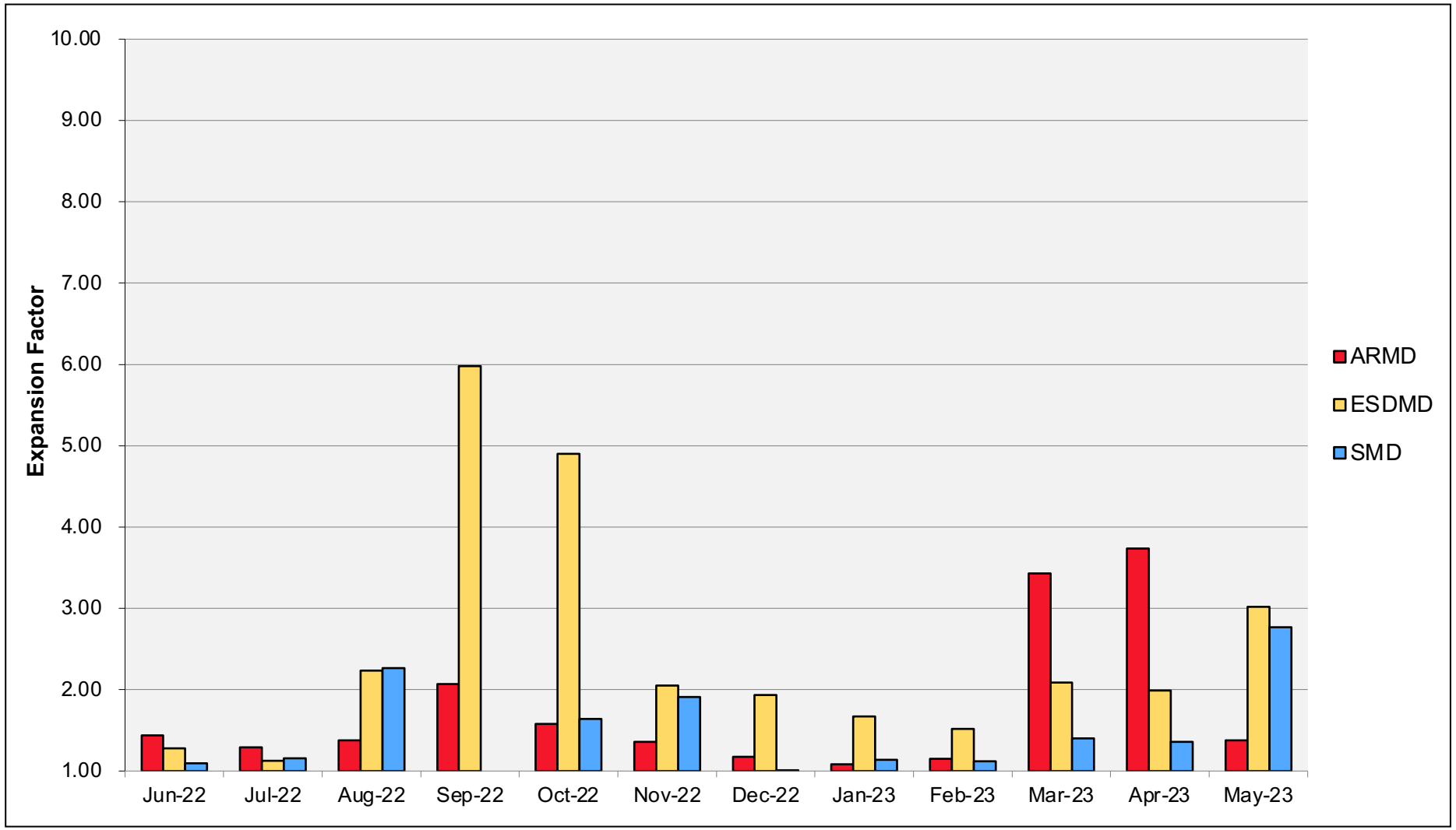
Aitken: Monthly Utilization by Size and Length



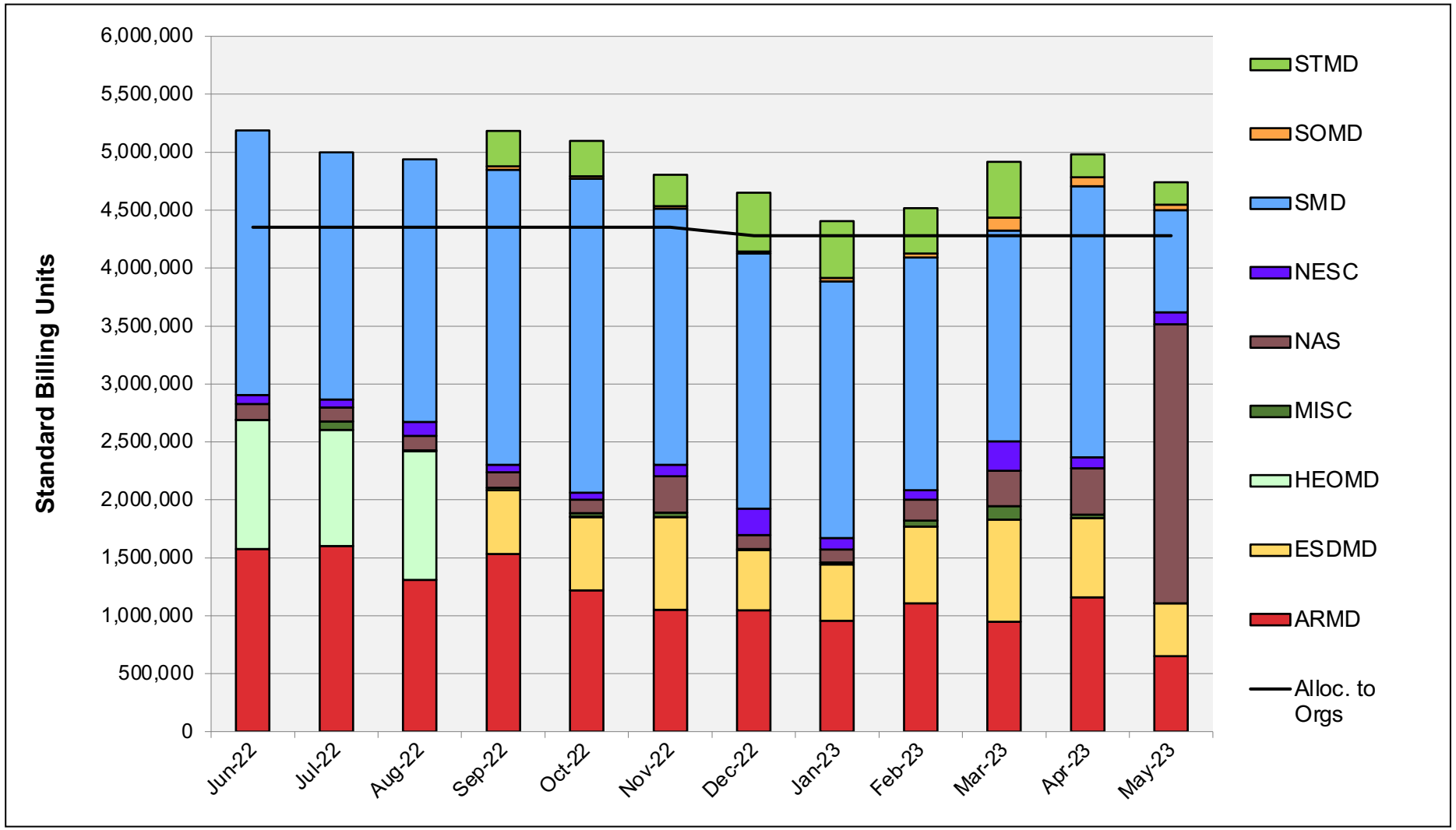
Aitken: Average Time to Clear All Jobs



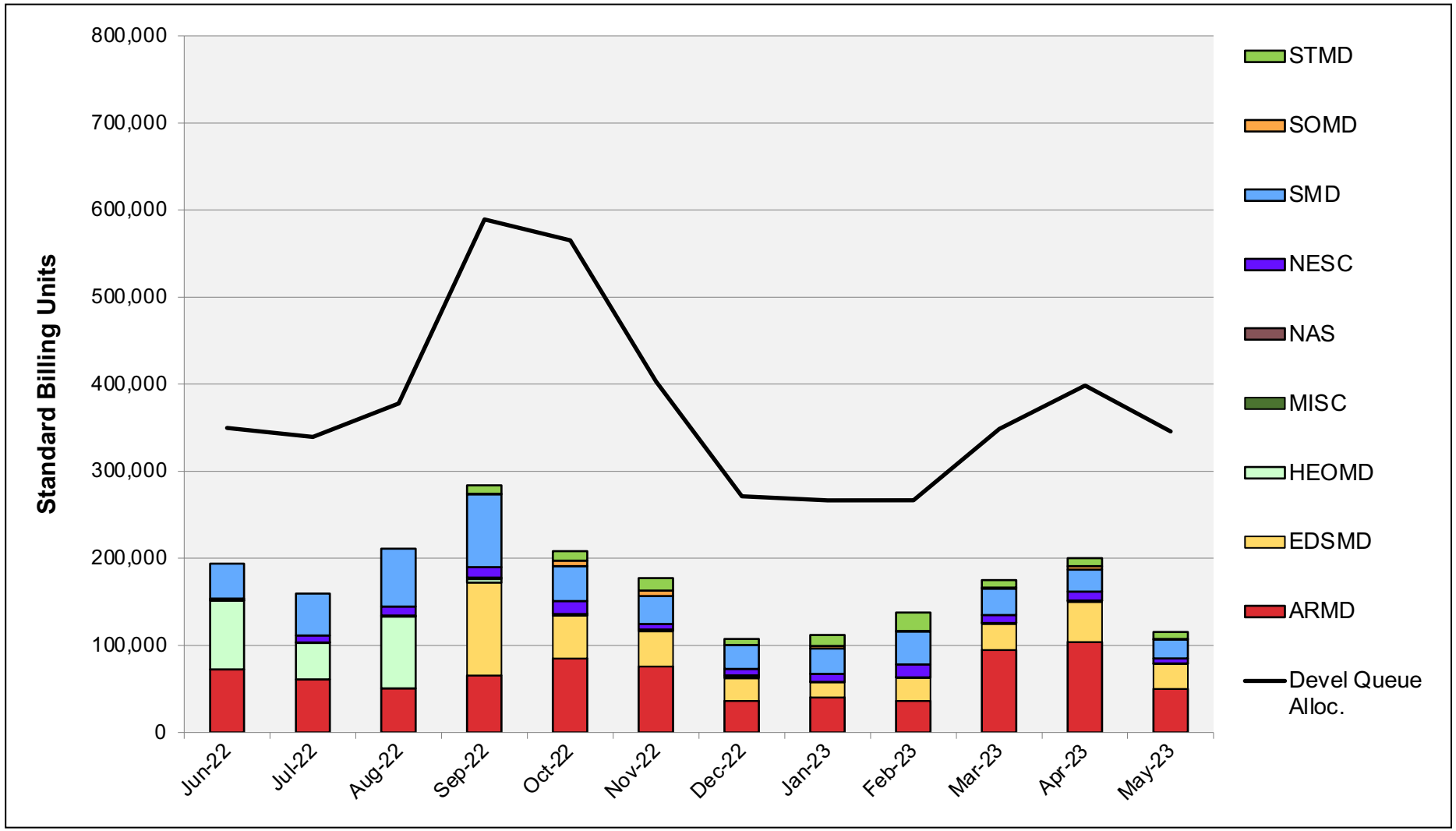
Aitken: Average Expansion Factor



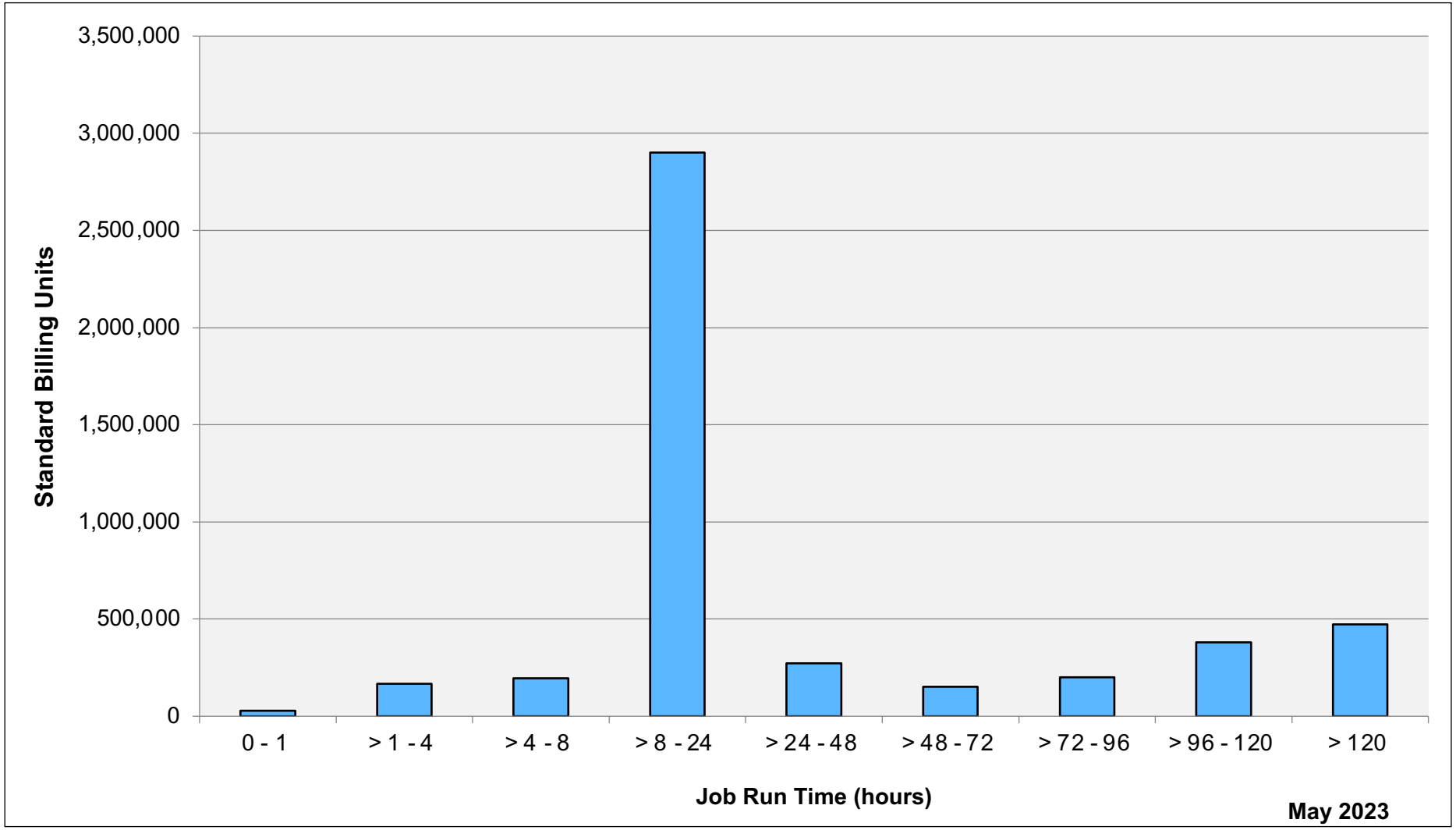
Pleiades: SBUs Reported, Normalized to 30-Day Month



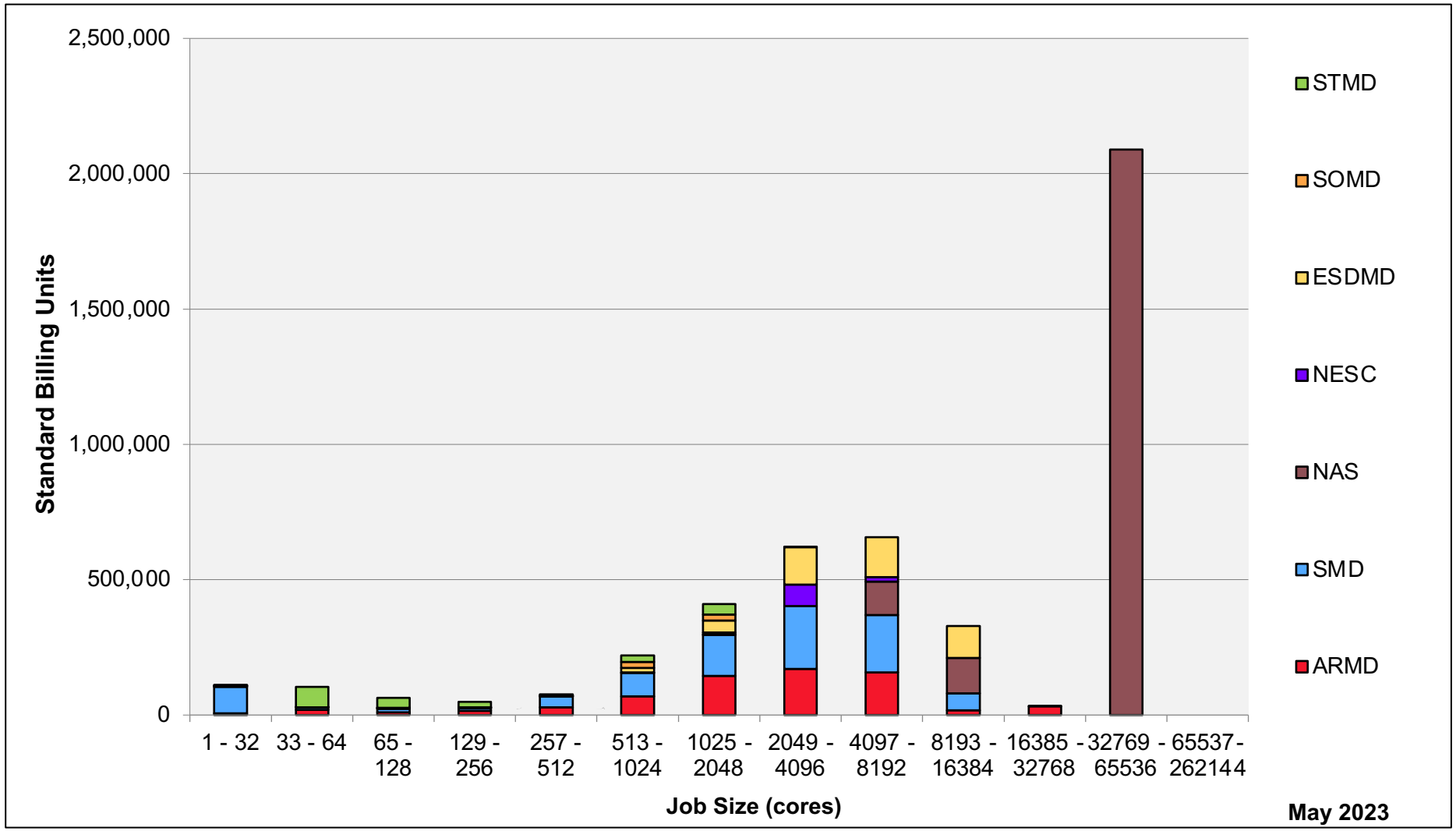
Pleiades: Devel Queue Utilization



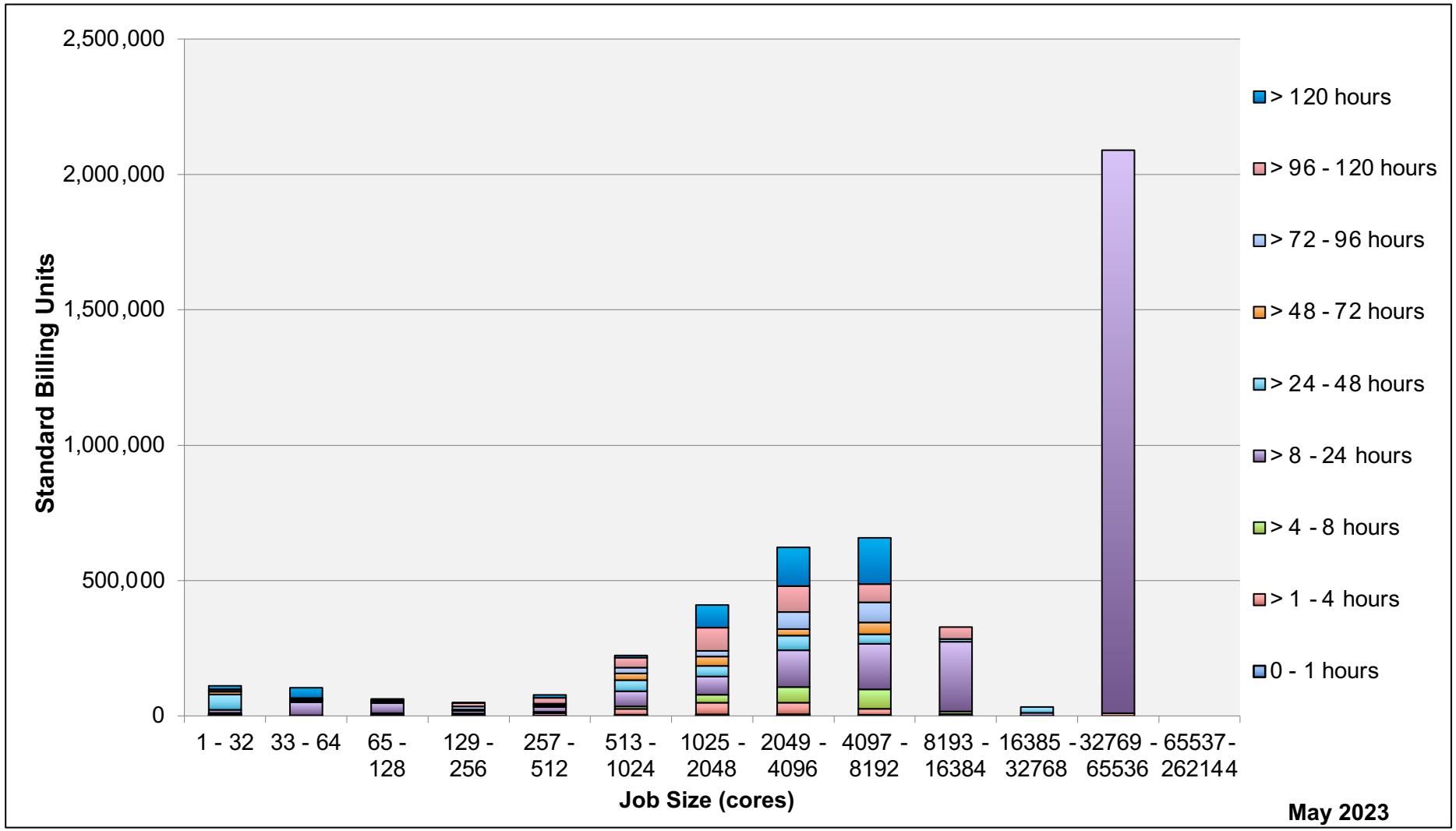
Pleiades: Monthly Utilization by Job Length



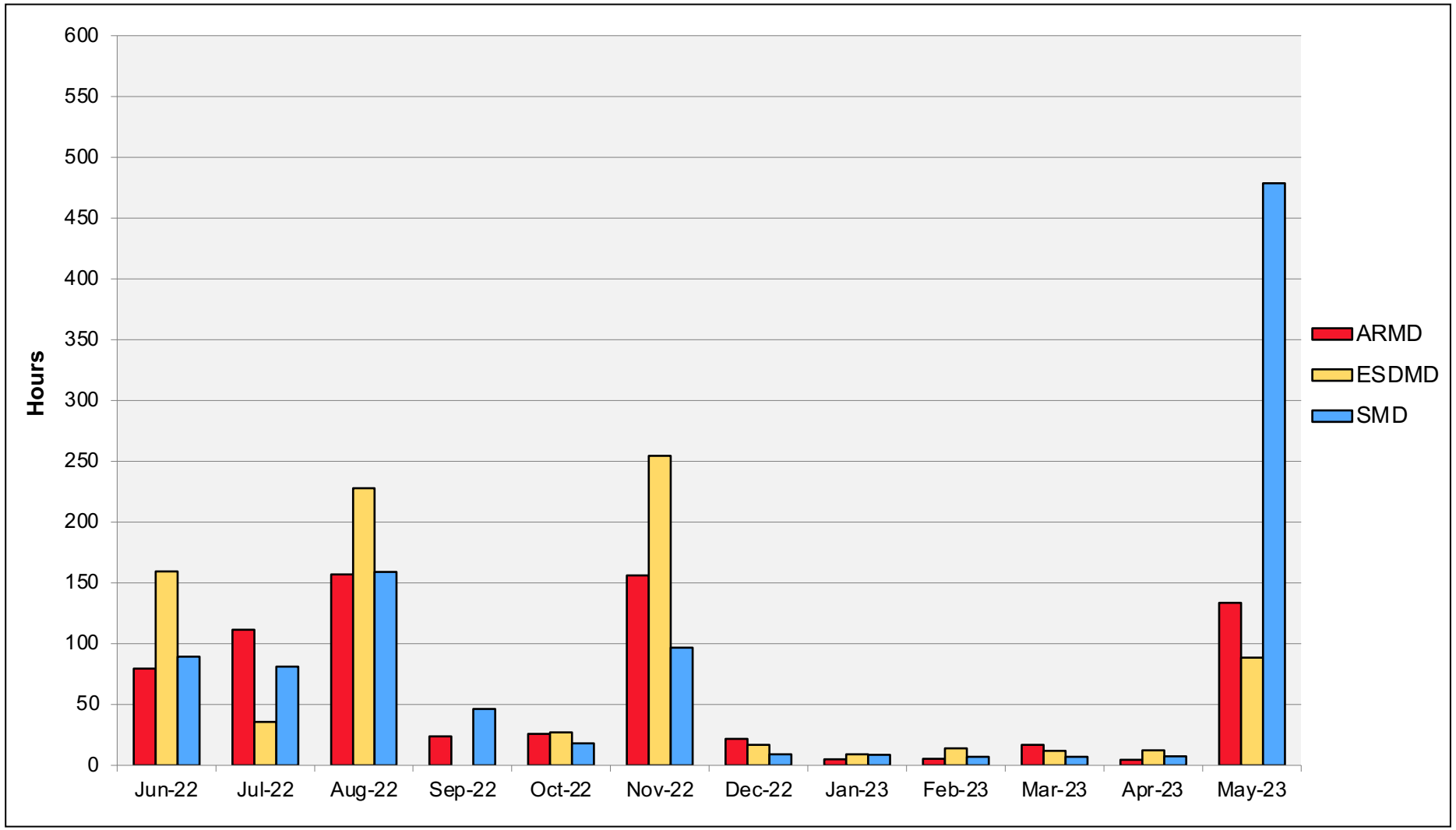
Pleiades: Monthly Utilization by Job Size



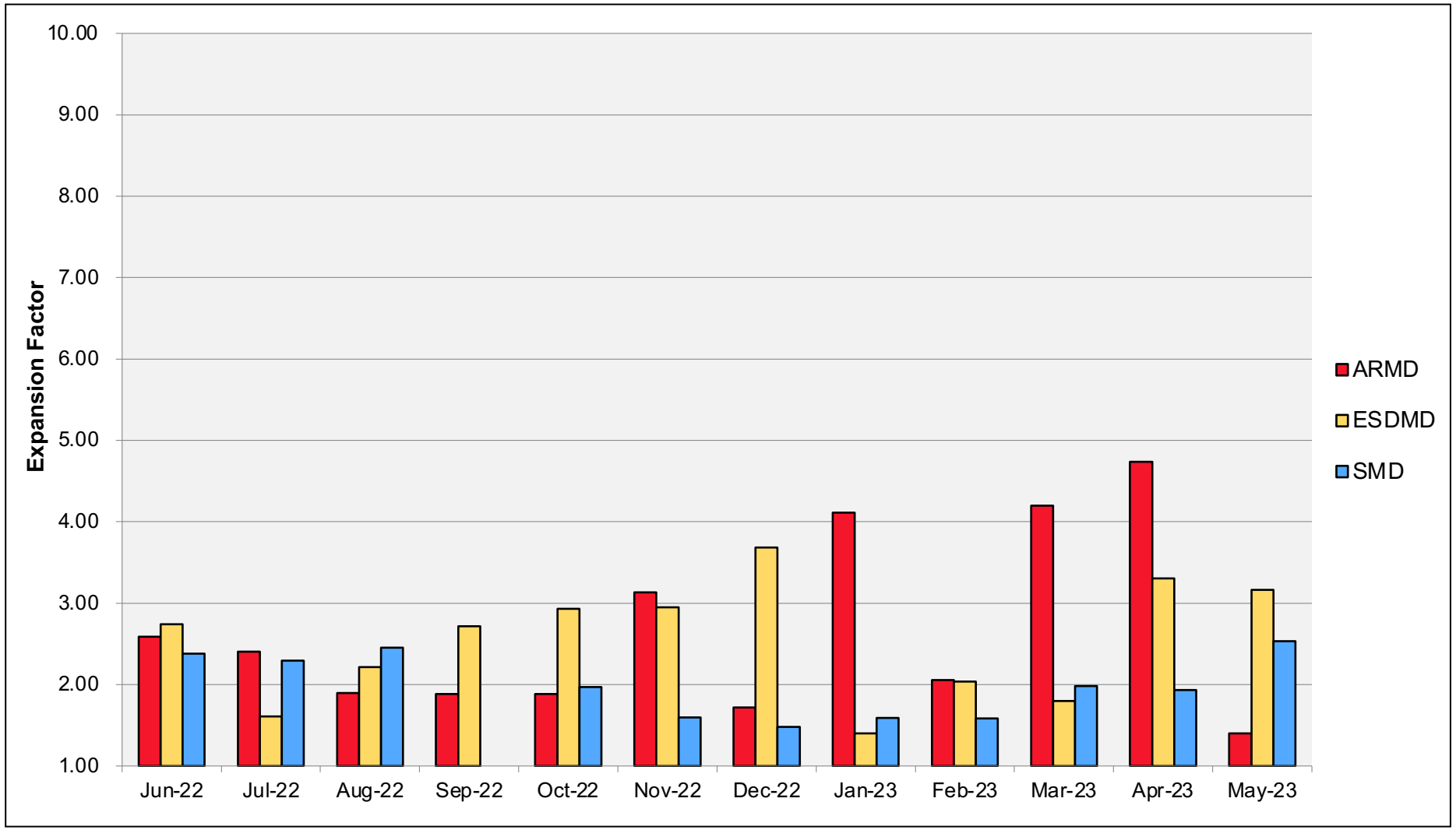
Pleiades: Monthly Utilization by Size and Length



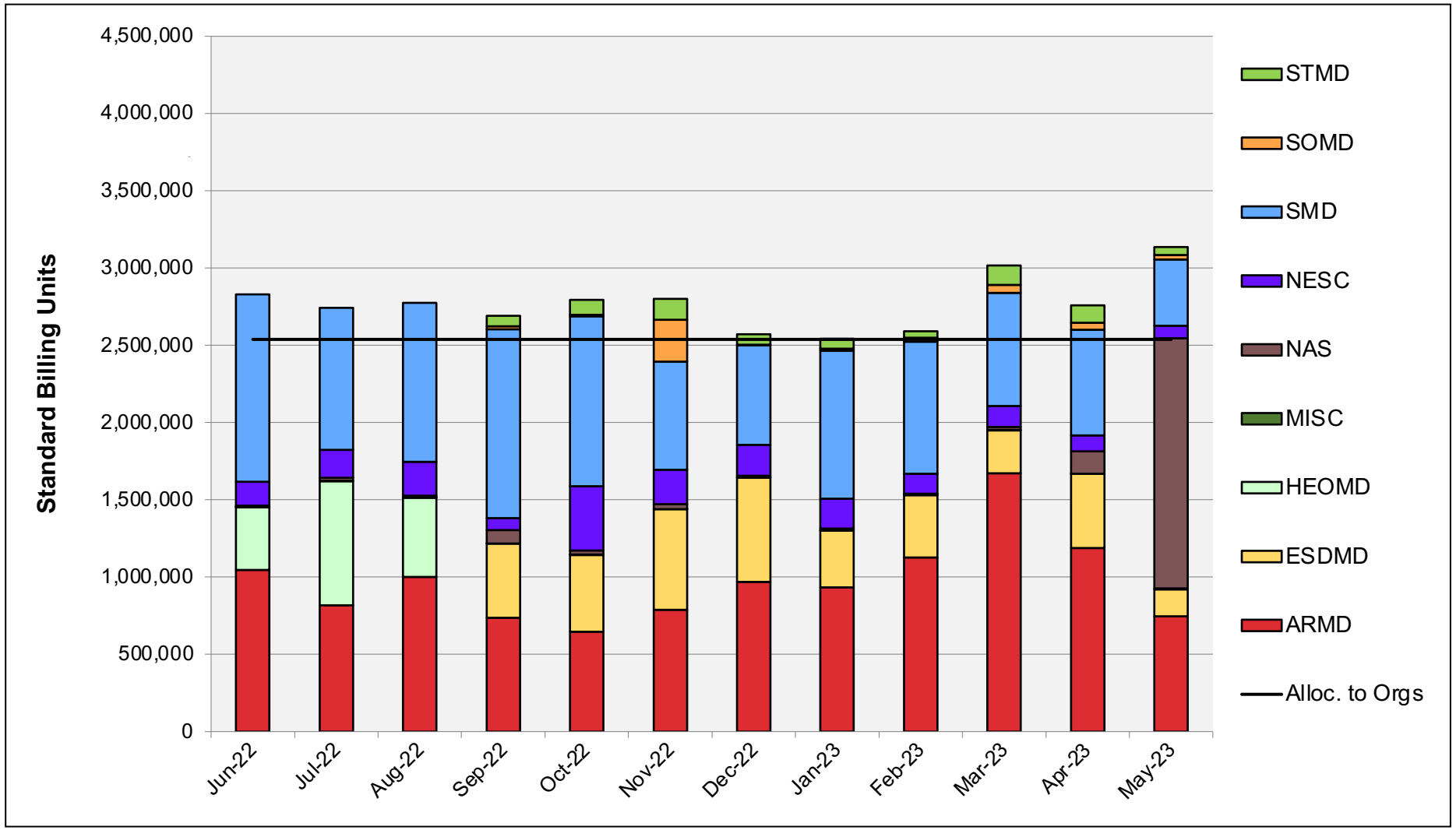
Pleiades: Average Time to Clear All Jobs



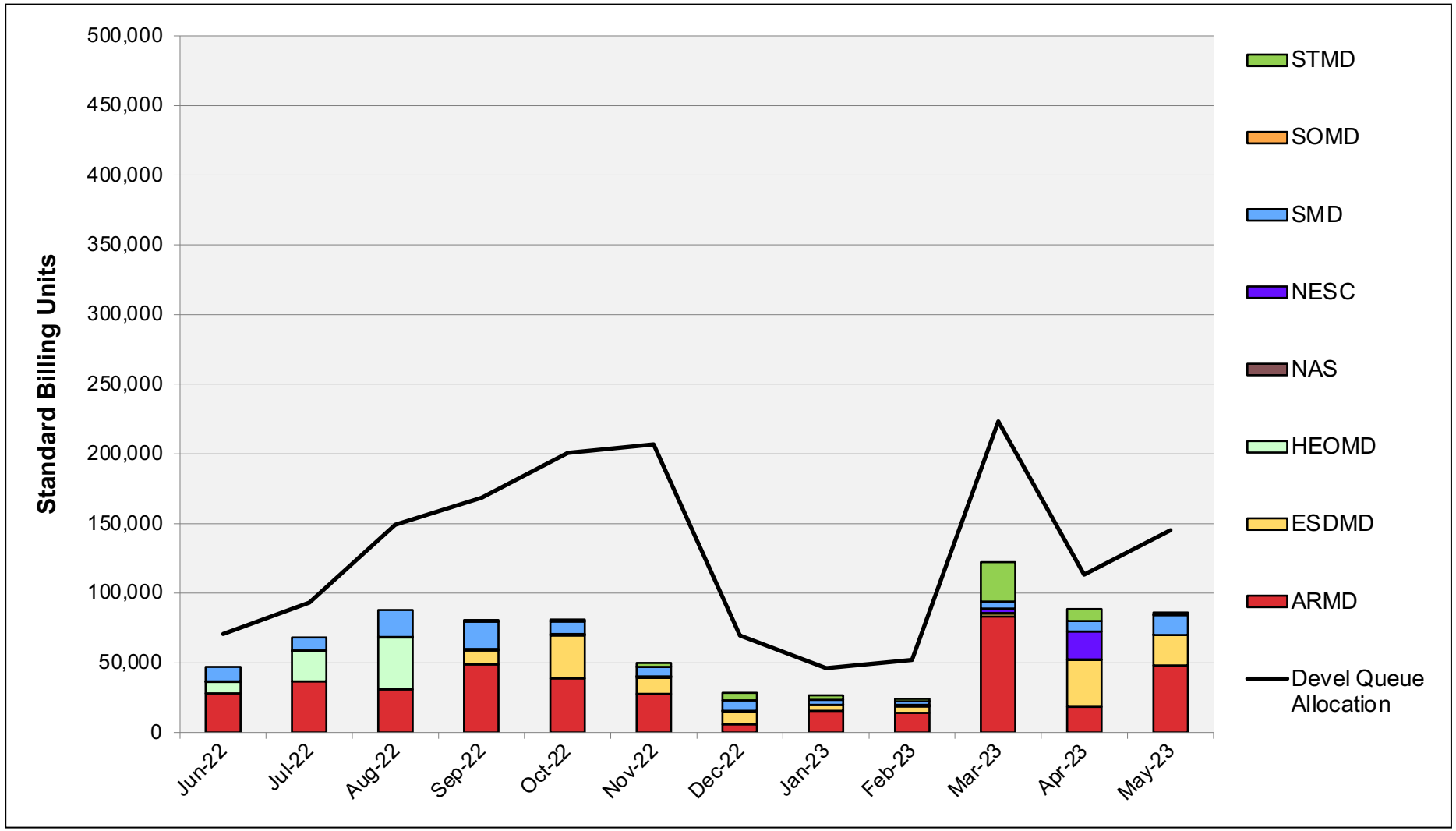
Pleiades: Average Expansion Factor



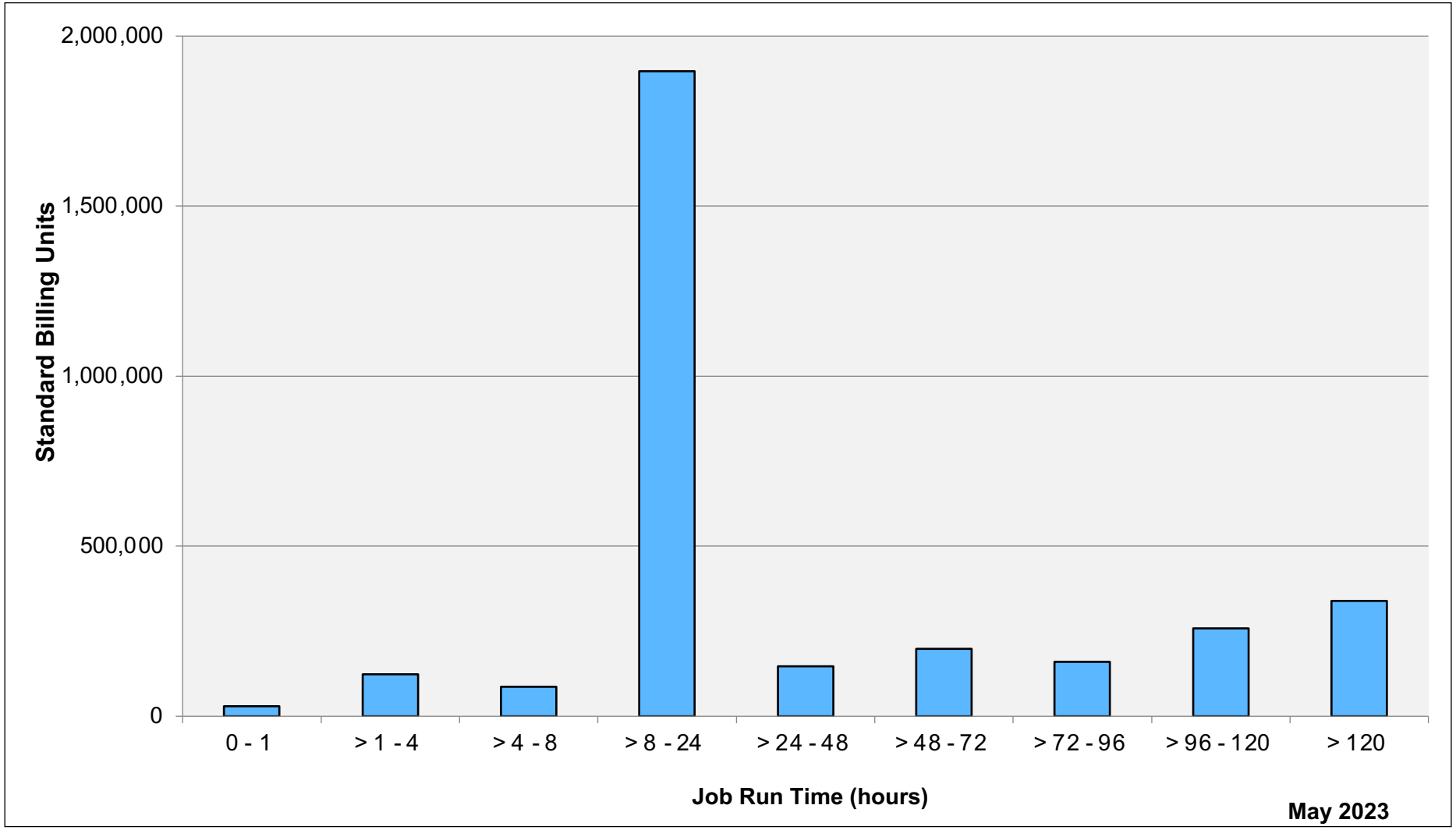
Electra: SBUs Reported, Normalized to 30-Day Month



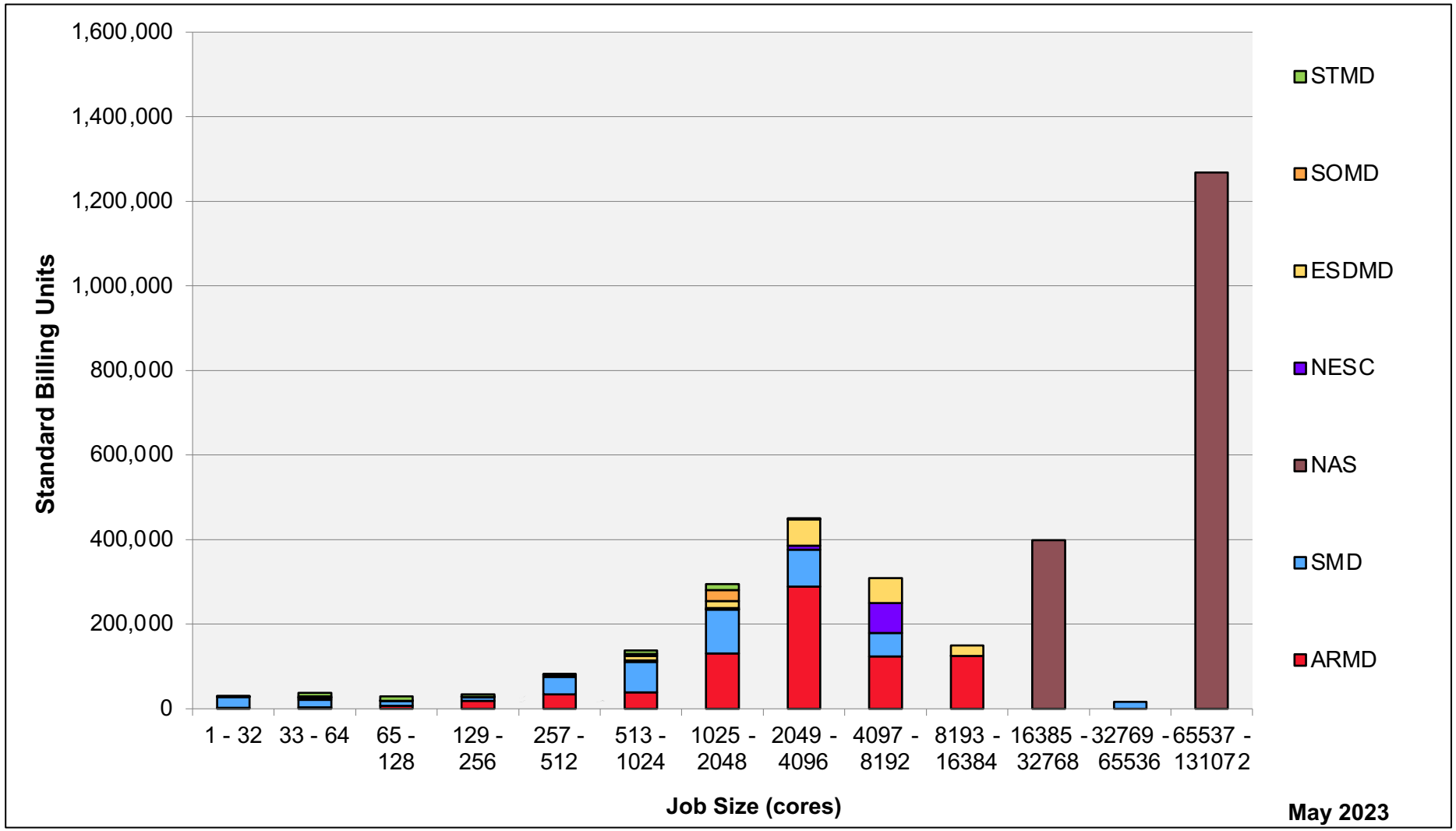
Electra: Devel Queue Utilization



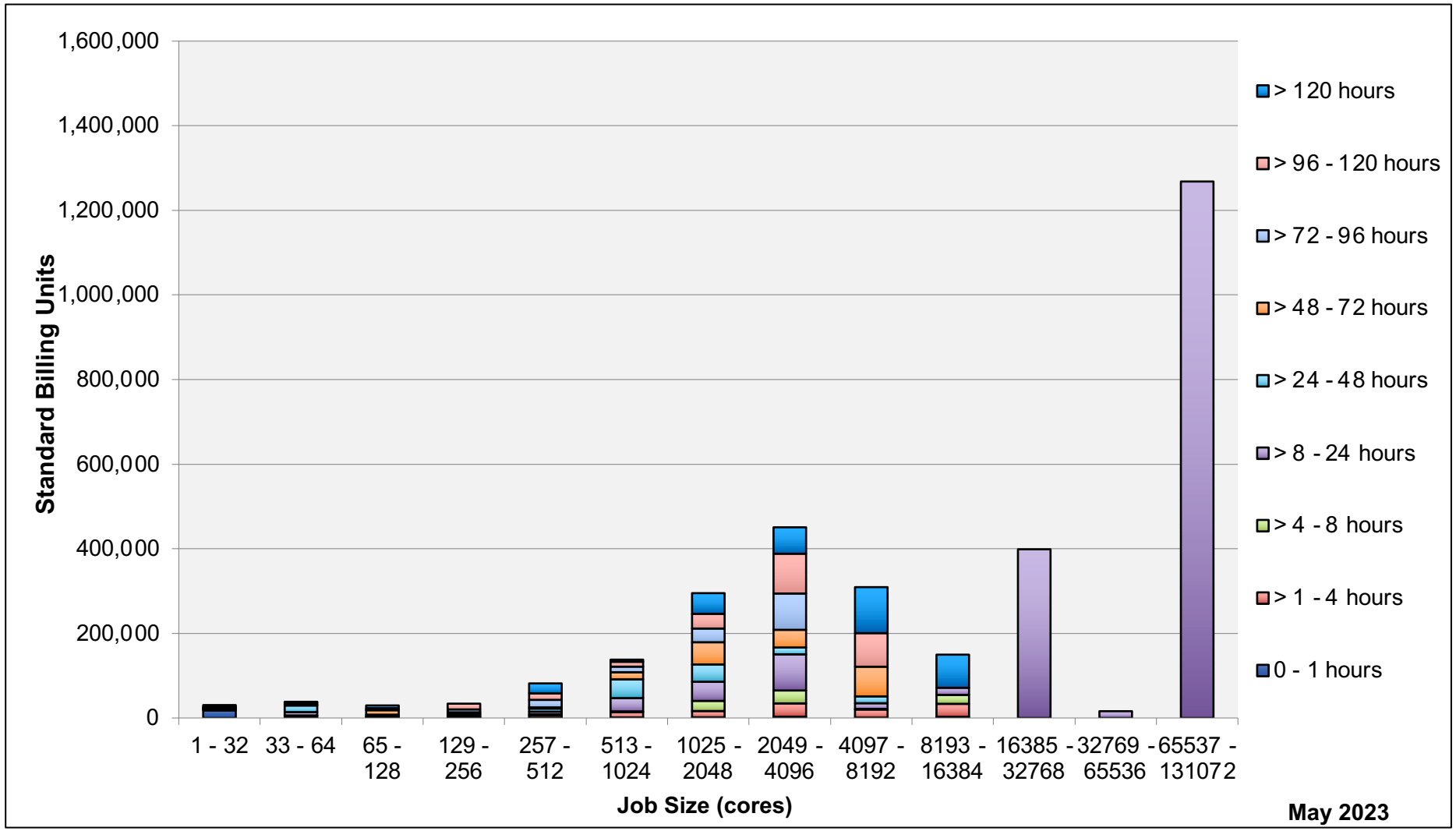
Electra: Monthly Utilization by Job Length



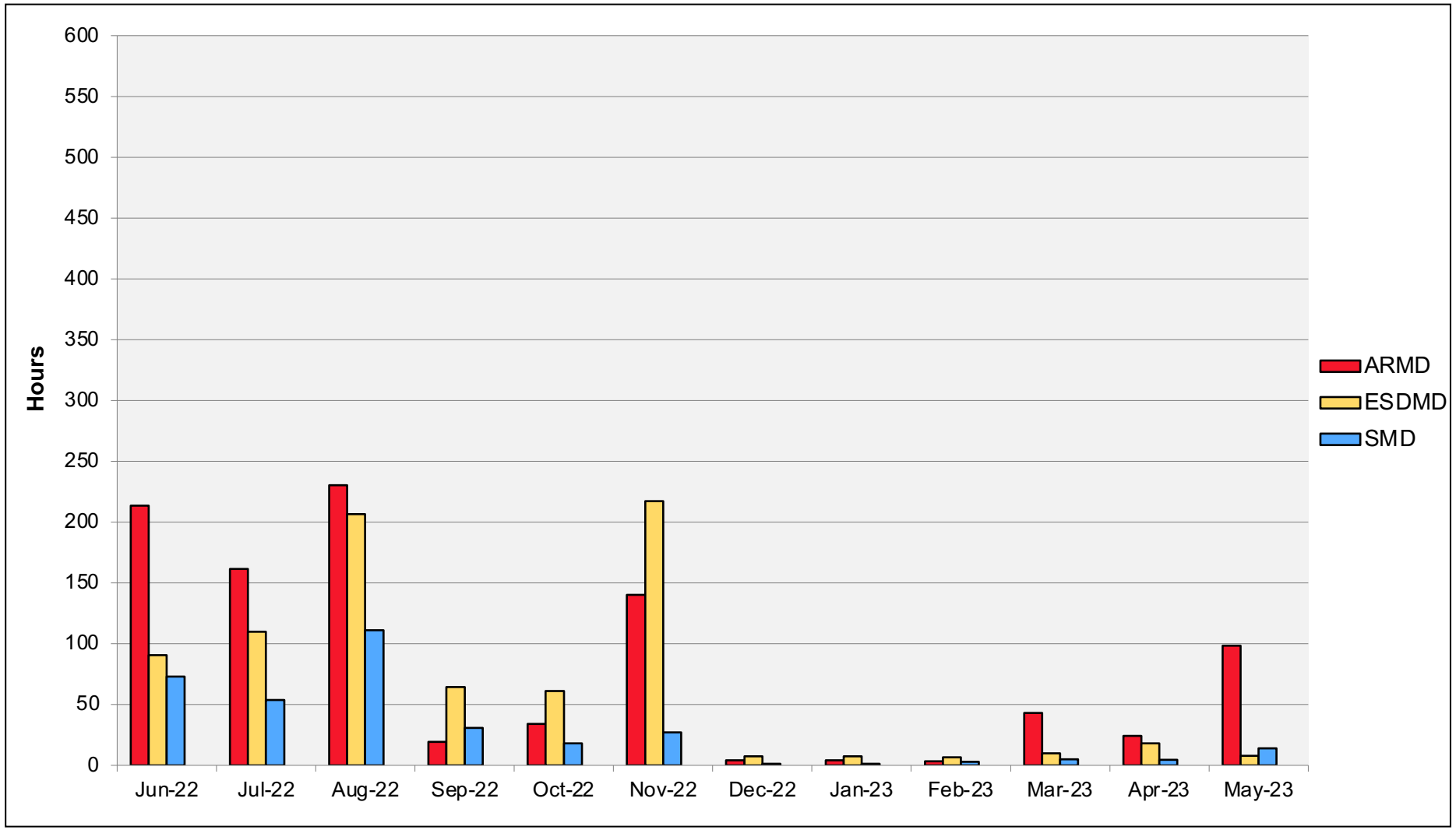
Electra: Monthly Utilization by Job Size



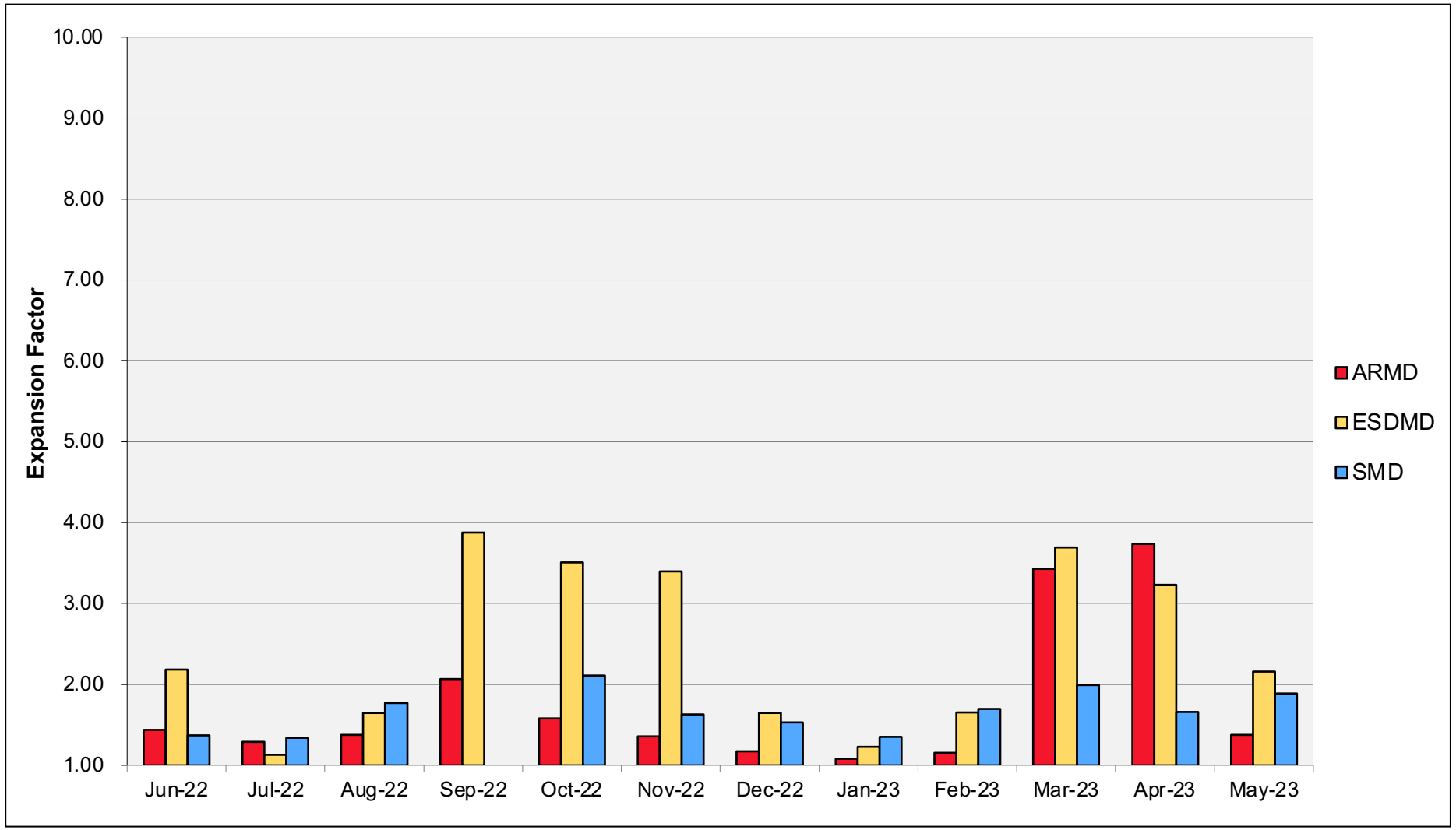
Electra: Monthly Utilization by Size and Length



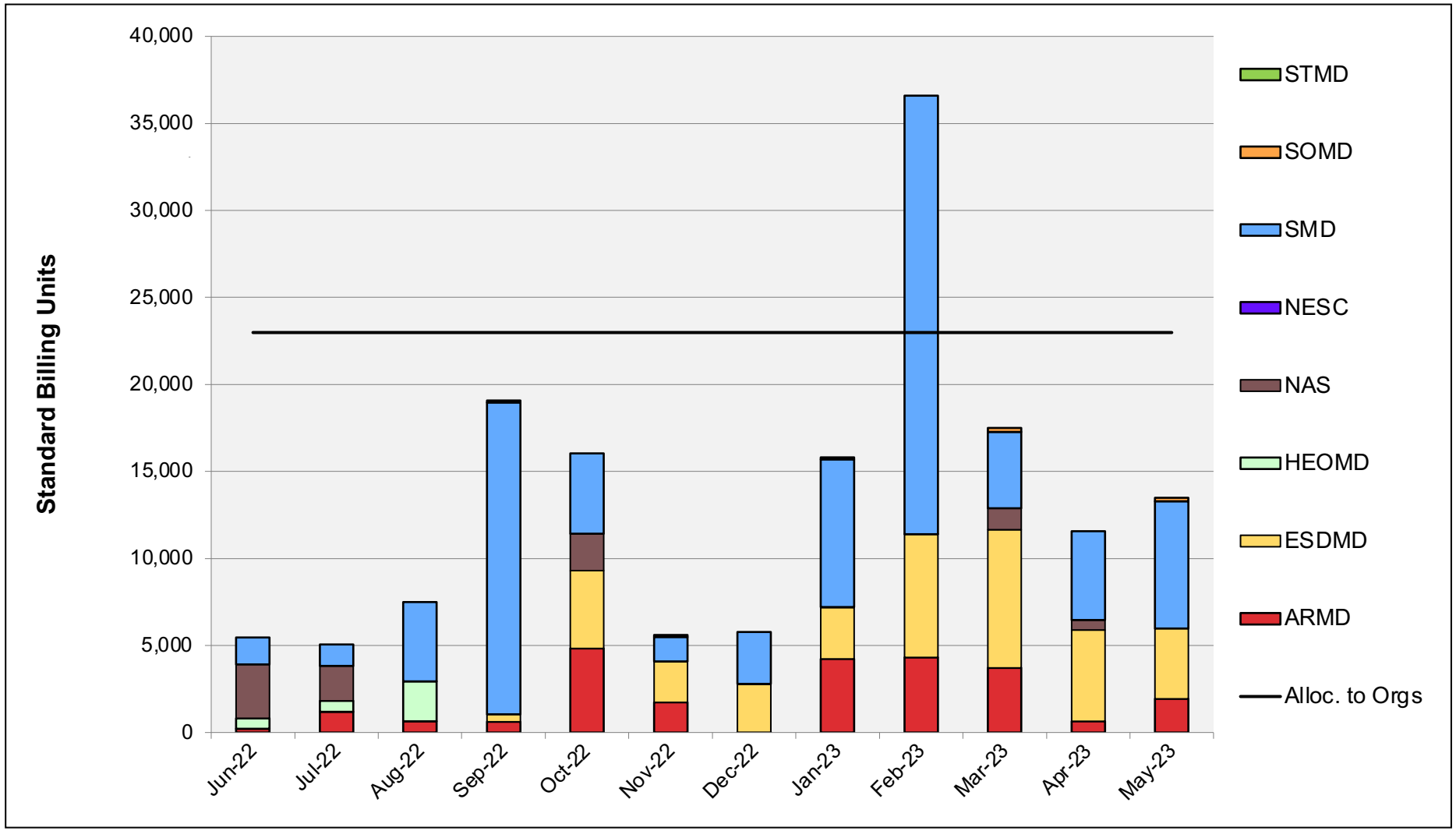
Electra: Average Time to Clear All Jobs



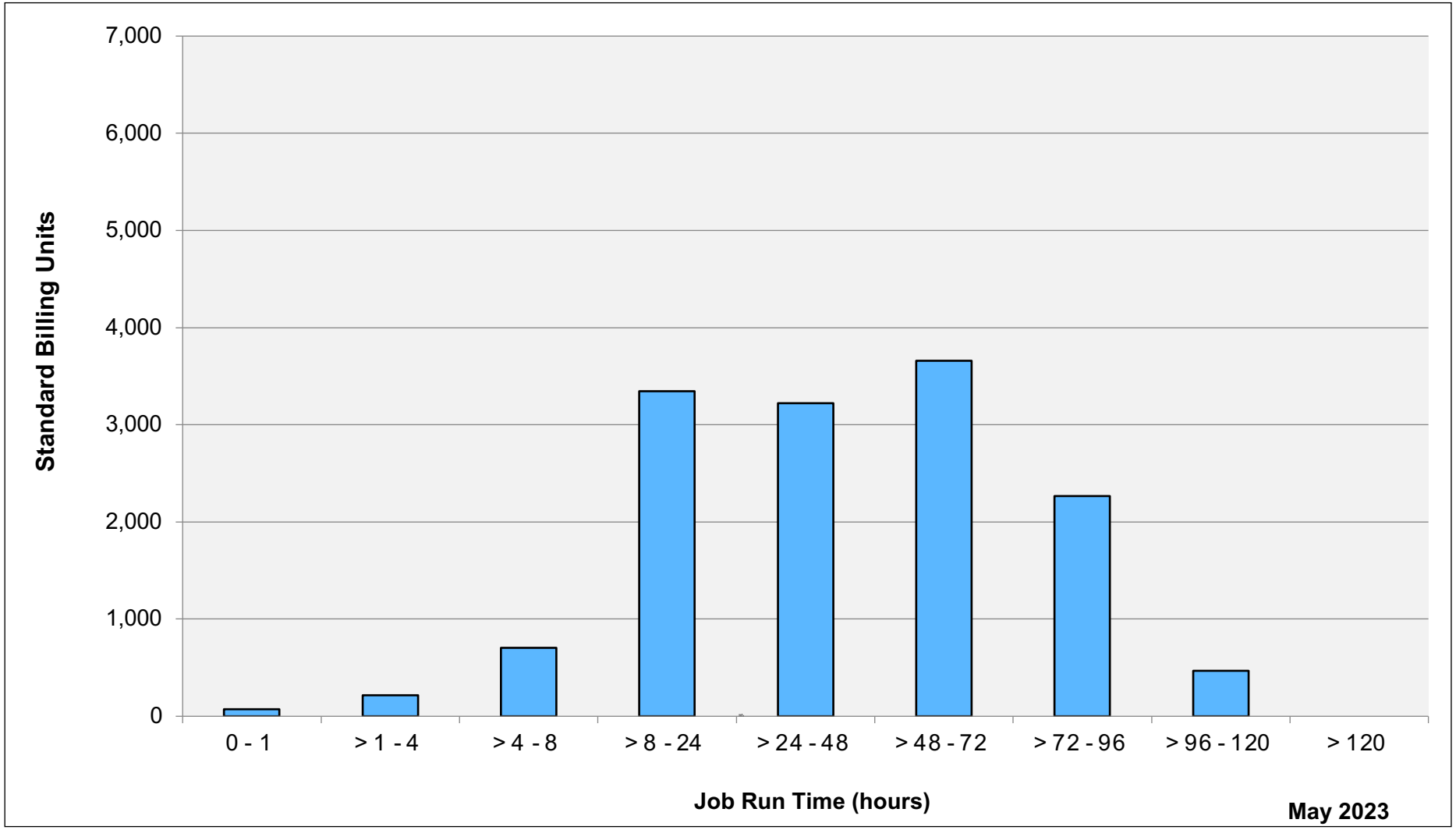
Electra: Average Expansion Factor



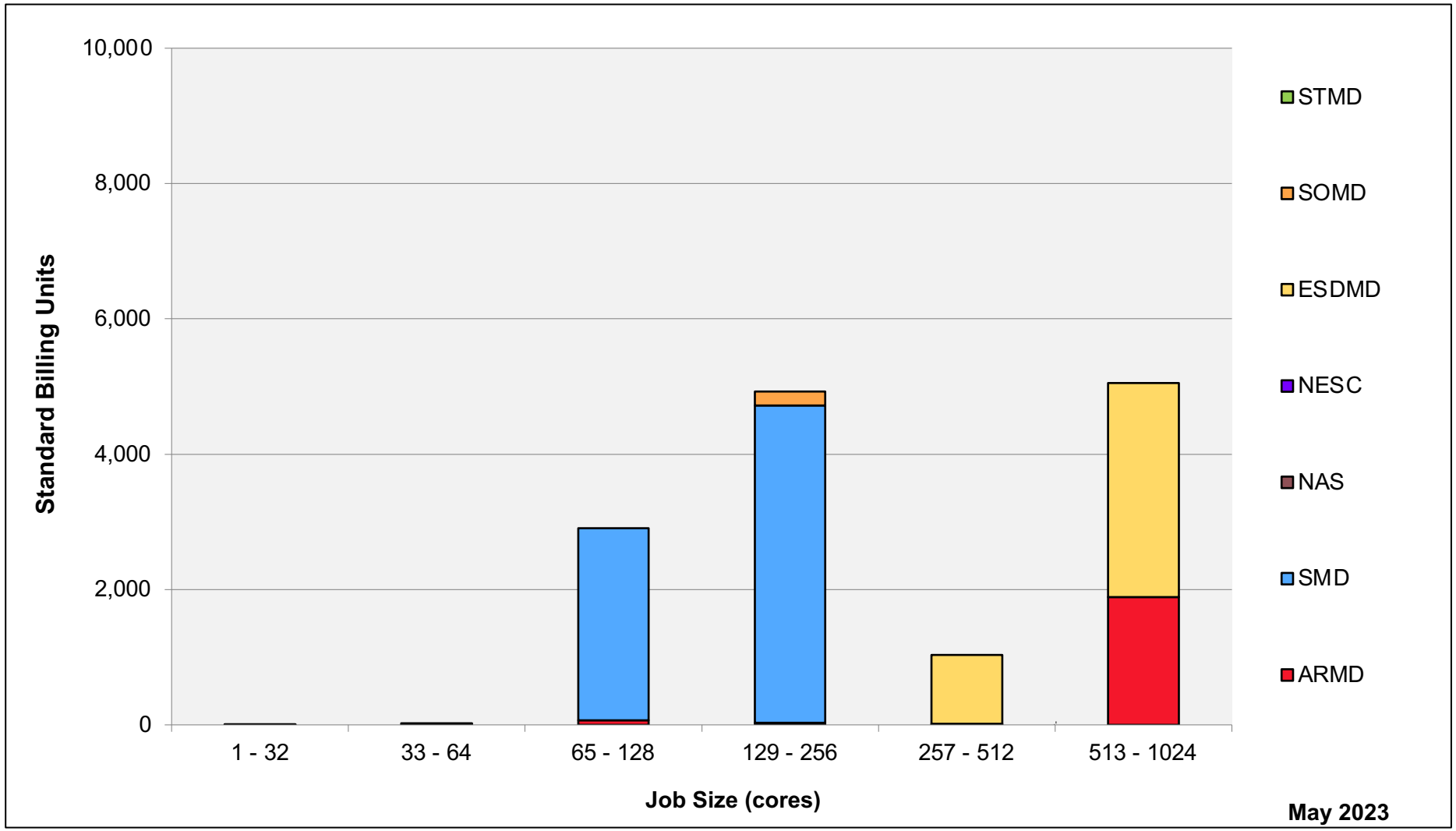
Endeavour: SBUs Reported, Normalized to 30-Day Month



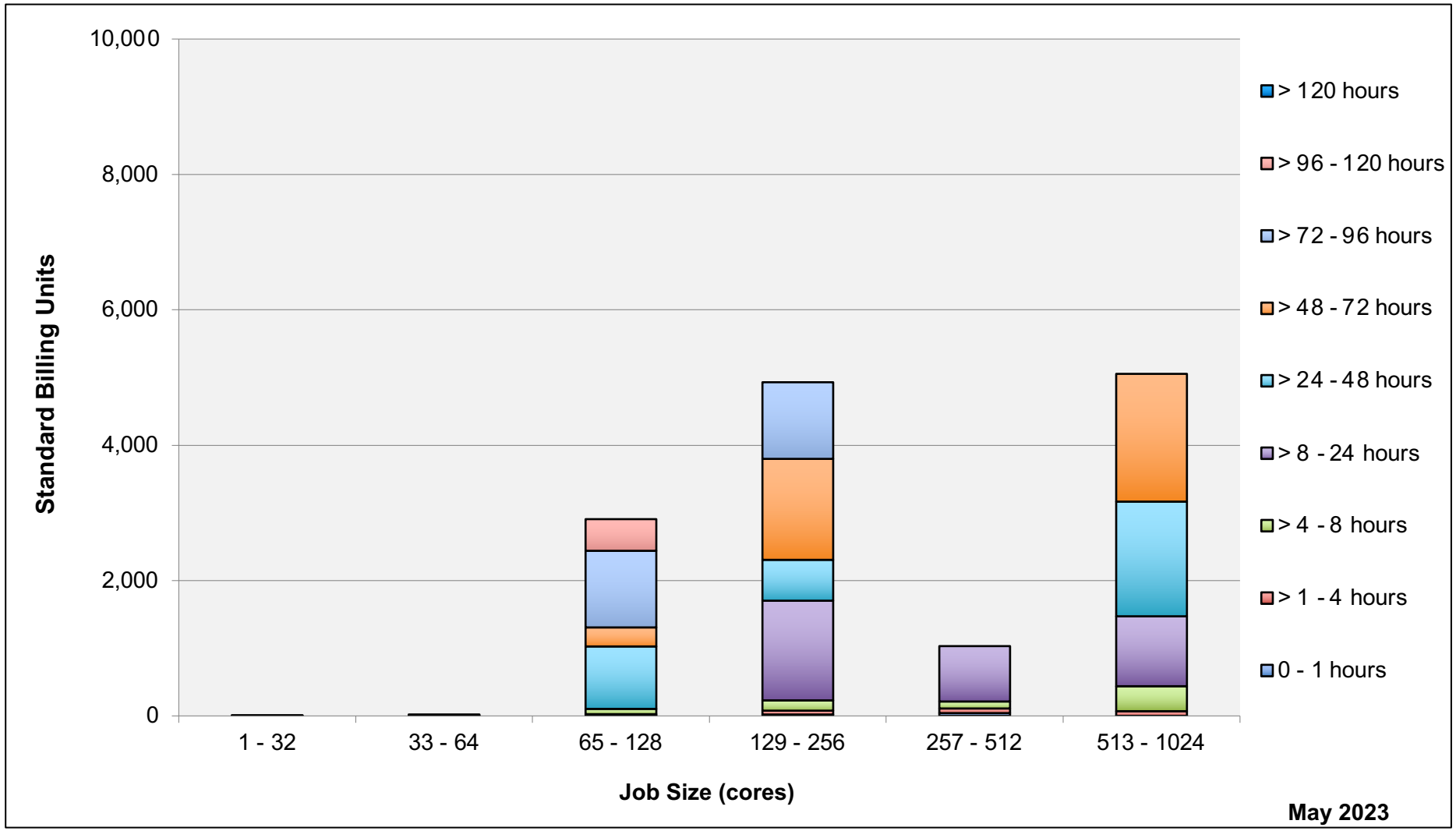
Endeavour: Monthly Utilization by Job Length



Endeavour: Monthly Utilization by Job Size



Endeavour: Monthly Utilization by Size and Length



Endeavour: Average Expansion Factor

