

National Aeronautics and Space Administration

High-End Computing Capability

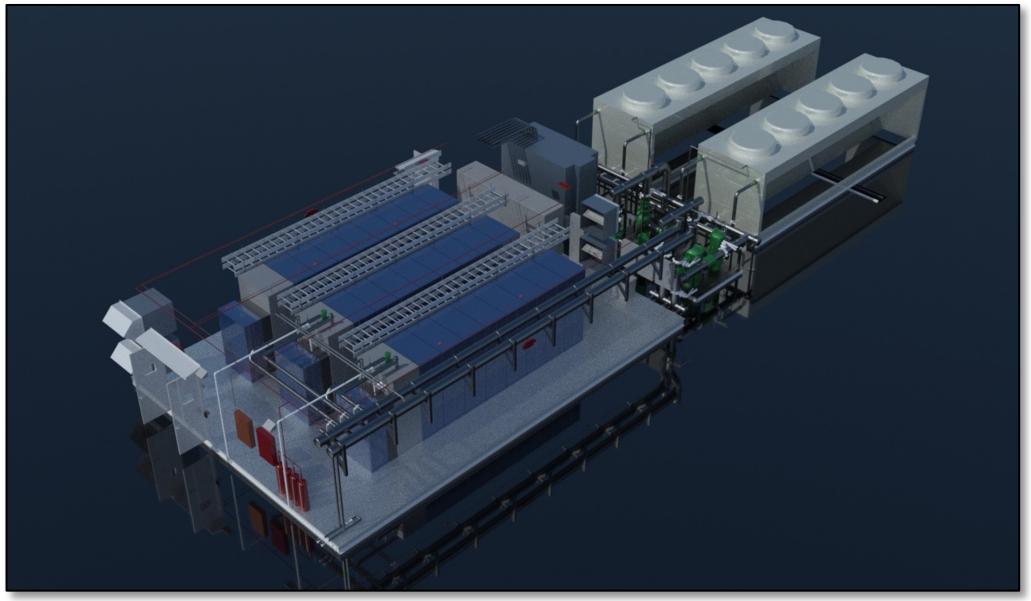
William Thigpen
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August 10, 2023

Milestone: 90% Design for MSF Compute Module 2

- HECC achieved an important milestone with the receipt of the 90% module design documentation package for the second compute module of the Modular Supercomputer Facility (MSF) at NASA Ames. This module targeted for the R&D099 site will support the expansion of the Aitken supercomputer.
- Module designer Avail Infrastructure Solutions (formerly AZZ, Inc.) delivered the 90% design of Compute Module 2 (CM2) on June 28, 2023.
  - The CM2 design package presents the site layout, interfaces to the existing compute module, module fire alarm and suppression, mechanical cooling equipment, electrical distribution, and building management system designs for submittal to the Ames Permit Board for a construction permit.
  - This design continues the environmentally responsible design philosophy of Compute Module 1 with no mechanical refrigeration (chillers) or recirculating cooling tower, reducing both energy and water usage when compared to a traditional data center facility.
- The Aitken expansion into CM2 will begin with HPE Apollo racks powered by AMD Milan processors. CM2 will provide three rows of compute racks at 1 megawatt per row, more than doubling the existing Aitken capacity.
- Avail Infrastructure is on schedule to deliver CM2 to NASA Ames in March 2024. Module and facility integration, plus facility commissioning, is projected to complete in June 2024.

IMPACT: Compute Module 2 supports the expansion of the Aitken supercomputer providing space for additional computing resources to the HECC user community.

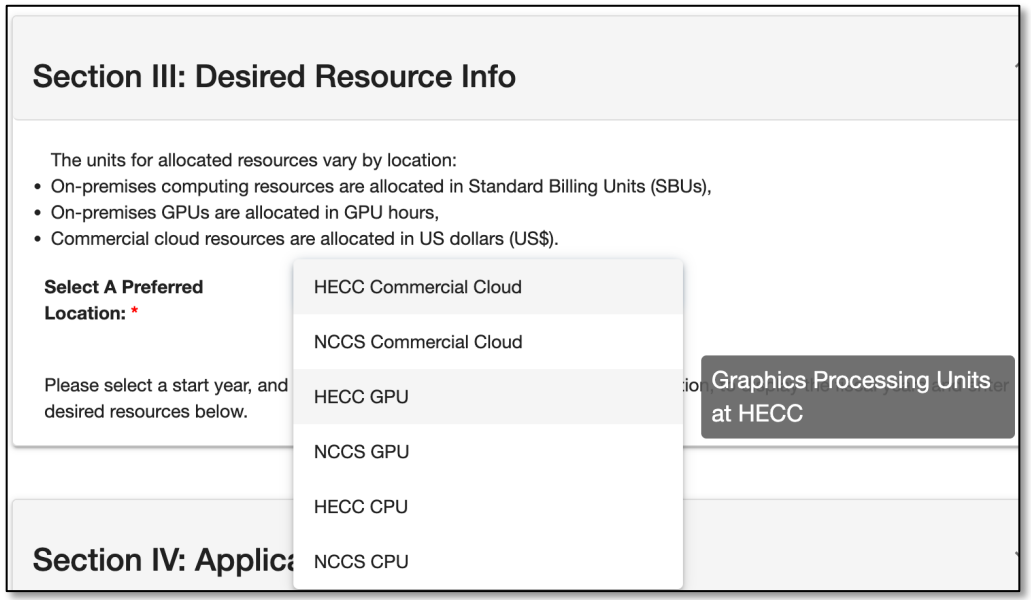


Compute Module 2 cutaway rendering showing the Aitken compute racks along with the mechanical and electrical infrastructure.
Avail Infrastructure Solutions

RMS Adds New Request Features

- Development of the Request Management System (RMS) application made significant progress through continuous integration, with two significant version releases in June and July.
- In June, RMS 3.7 added the mandatory Space Technology Mission Directorate (STMD) Portfolio Analysis Resource (SPAR) ID. The SPAR ID is the unique record identifier for the STMD technology development project in the SPAR database.
  - The SPAR ID is critical to confirming eligibility of the STMD project.
  - The SPAR ID is only shown if a PI selects STMD as the Mission Directorate.
  - The new functionality for STMD was demonstrated to Karen Knight, STMD HECC Representative, with fellow SPAR Quality Data Analysts from Headquarters.
- RMS 3.8 introduced the ability to request NCCS or HECC GPU resources.
  - The "Desired Resource Info" section was changed from radio buttons to a dropdown, with helpful text defining the units for allocation (*see screenshot*).
  - Generates PDFs for users requests.
- The call for the GPU new operational period (NOP) was released on Tuesday, August 1, 2023 and will close Friday, August 25, 2023.
- Upcoming RMS versions will focus on the administrative side of GPU requests, such as updating view pages, notifications for GPU requests, and Admin UI for allocating GPU resources.

IMPACT: Developing in-house software to manage supercomputer resource allocation requests allows NASA's High End Computing Program more ownership of the data, and simplifies the process for reviewing allocations and targets.



Screenshot of new dropdown selection box listing available resources to request in the Request Management System.

HECC Completes Annual Building Maintenance

- HECC facilities engineers, in collaboration with Code J, Jacobs Engineering, and HPE, planned, coordinated, and conducted the annual building maintenance for N258, R&D088, and R&D099. The work included numerous repairs and maintenance of key components of the facilities.
- Building N258 and the Modular Supercomputing Facility (MSF) site maintenance required complete power shutdowns. The Pleiades, Electra, Aitken, Endeavour, hyperwall and storage systems were all powered off.
- Maintenance activities completed:
  - Cleaned the N258 cooling tower, chiller condenser tubes, and computer room subfloor.
  - Cleaned the MSF R&D099 high-voltage switchgear and adiabatic coolers.
  - Cleaned and tested 480V switchgear and circuit breakers. Tightened branch circuit electrical connections that were operating warm during a pre-shutdown infrared scan.
  - Replaced belts and filters on the building and computer room air handlers.
  - Tested all N258 fire suppression systems.
- In addition, the Facilities team installed new utility-grade power meters for R&D088 and R&D099 to measure site energy usage.
- They also installed a new in-rack cooling unit in the Electra Skylake I/O rack to provide redundant cooling for the Electra rack leaders.

IMPACT: Preventative maintenance on the HECC facilities' cooling systems and electrical distribution is essential to eliminate downtime caused by aging infrastructure, yielding more computer uptime for NASA science and engineering users.



High-voltage specialist electricians from Jacobs Engineering reinstall a vacuum circuit breaker in its enclosure.
Chris Tanner, NASA/Ames

Optimization and MPI Parallelization of cubep Application

- The HECC Application Performance and Productivity (APP) team optimized and parallelized the cubep ab initio quantum chemistry code, which is used by the HECC Visualization team to generate further numerical data from ab initio output files.
  - As problem sizes increase, there is a need for faster processing.
  - The code, which is parallelized using OpenMP, evaluates the electronic charge density on a user-specified lattice of sample points associated with a molecular structure.
- The APP team performed the following techniques:
  - Employed dynamic work scheduling for OpenMP parallelization. This reduced workload imbalance and improved the performance by approximately 1.2 times.
  - Added a 1D MPI parallelization to the OpenMP code using an embarrassingly parallel approach that does not require domain composition. No data communication is required, but IO requires synchronization of the MPI processes.
- With these improvements, the MPI+OpenMP parallel code now allows processing of large 3D cubes in an acceptable time.
  - Using 1 MPI rank + 32 OpenMP threads on a cube of size 256^3 takes 4258 seconds on a single Skylake node. On 8 nodes using 8 MPI ranks and 32 OpenMP threads per rank, the processing time decreases to just 580 secs.

IMPACT: The optimized MPI+OpenMP parallel code allows processing of large 3D cubes in an acceptable time to be used within a visualization workflow.

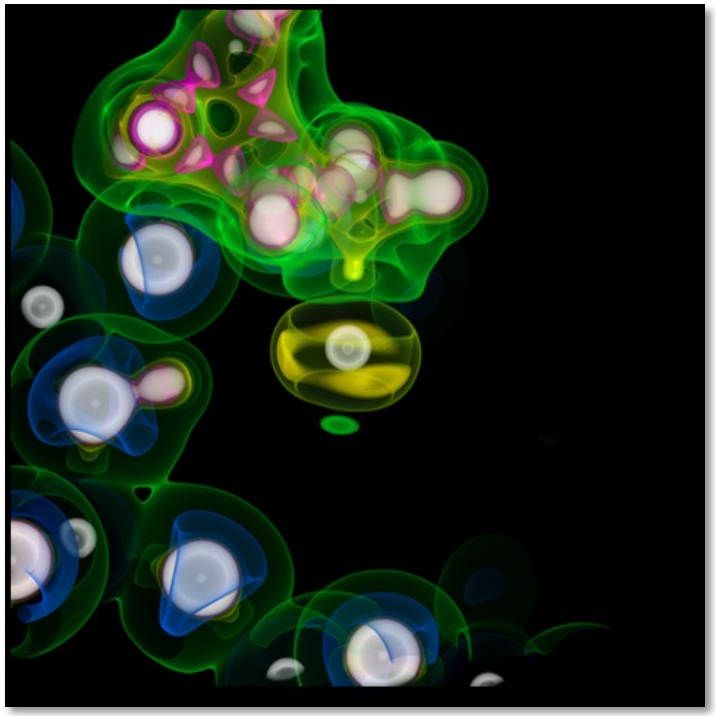
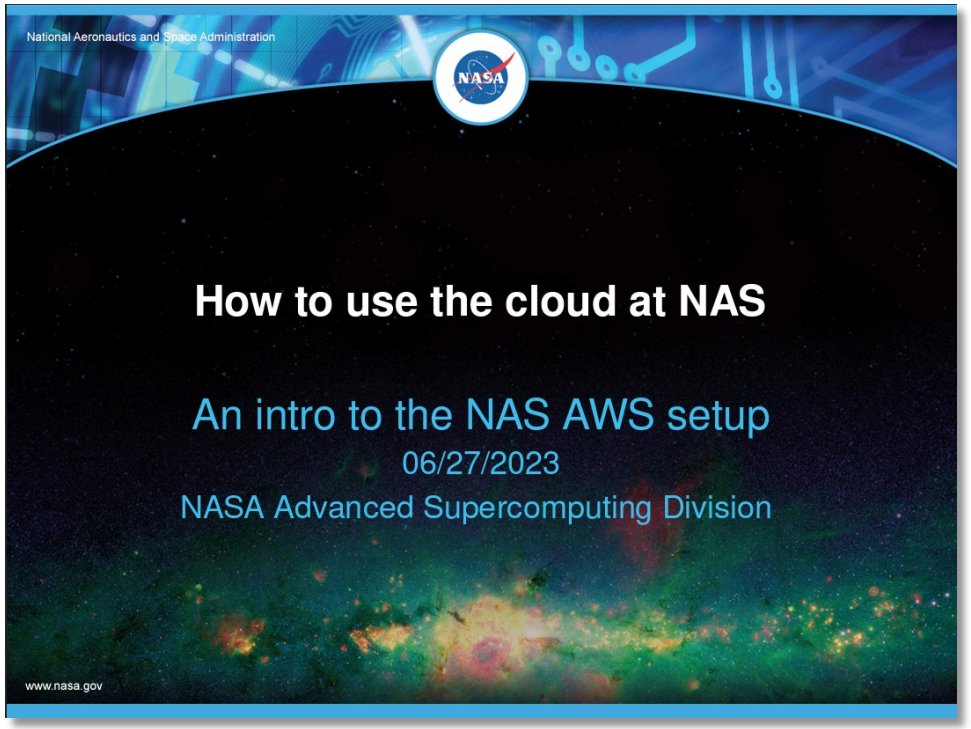


Image resulting from work on controlled reactions using brominated cyclopropane in a zeolite, using the cubep code. *Visualization Team, NASA Ames*

Cloud Team Presents AWS Environment Webinar

- On June 27, the HECC Cloud team conducted a user training session, “How to Use the NAS AWS Cloud,” detailing the current HECC cloud offerings.
- The webinar contained an overview, lessons learned, and best practices on how to work with the Amazon Web Services (AWS) environments.
- The training session also demonstrated how to sign up for cloud access using the Request Management System (RMS), and where to find documentation in the HECC Knowledge Base.
- The content was well received, and attendees asked many excellent questions during the Q&A session of the talk.
- A pre-recorded webinar and slides were posted on the HECC website for all users to access.
  - https://www.nas.nasa.gov/hecc/support/past_webinars.html
- The Cloud team will continue to monitor trends and issues experienced by the user community. If beneficial, a follow-on webinar will be developed to keep the NAS user community informed.

IMPACT: Providing knowledge of how to access available cloud resources and support services enables the HECC userbase to transition to these resources when needed.

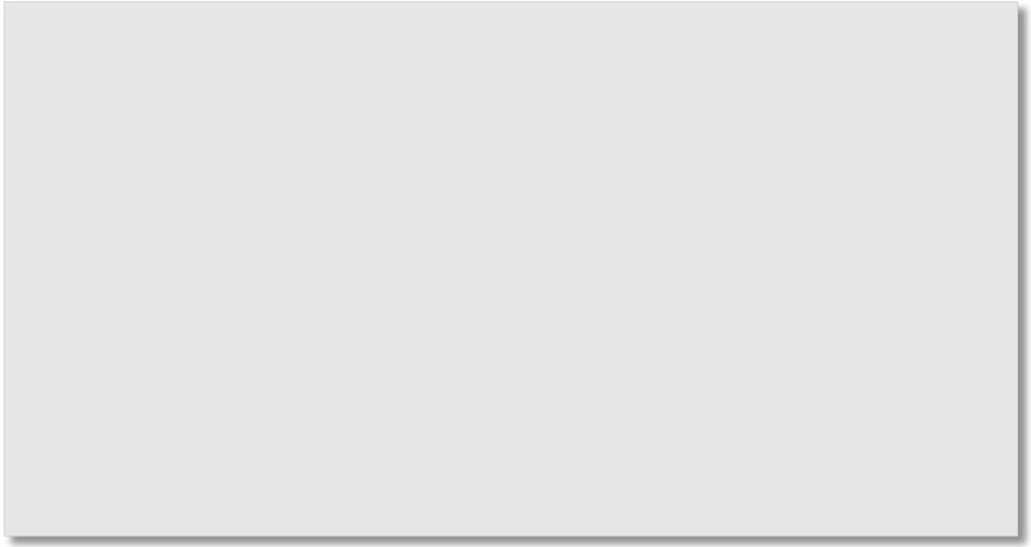


Title slide from the AWS webinar, which informed the HECC user community of available cloud capabilities and how to use the NAS cloud resources.

A New Strategy for Ensemble Seasonal Forecasts*

- Researchers at NASA's Global Modeling and Assimilation Office (GMAO) produce seasonal forecasts on a monthly basis. Because seasonal forecasts are an inherently "noisy" endeavor, many individual forecasts must be run to produce an ensemble forecast.
- Using the Aitken supercomputer, the GMAO team developed a new computational strategy to conduct these ensemble forecasts, ensuring that an ensemble properly spans the range of possible forecasts. The new "Synchronized Multiple Time-lagged" (SMT) approach allows the team to generate a reliable and computationally efficient suite of retrospective forecasts.
- The researchers created a retrospective suite of forecasts that runs for each month from 1992 to 2022 (for 30 years, or 360 initial condition months). Each month of forecasts includes 40 three-month runs, and another 10 that run for an additional six months, resulting in 180 simulated months for each month of forecast initial states.
- SMT was included in the most recent version of the Goddard Earth Observing System's Subseasonal to Seasonal Prediction system, GEOS-S2S-3, and will help provide reliable seasonal and subseasonal forecasts to a wide range of users—from agricultural to health and military sectors.

IMPACT: The SMT approach improves the prediction skill of the GEOS ensemble, providing NASA and other scientists with the tools to study seasonal forecasting and use them to advance the ability to make long range, societally relevant predictions.



Video demonstrating a portion of NASA GMAO's Synchronized Multiple Time-lagged (SMT) approach to producing seasonal/subseasonal ensemble forecasts. *Andrea Molod, Sterling Spangler, NASA Goddard*

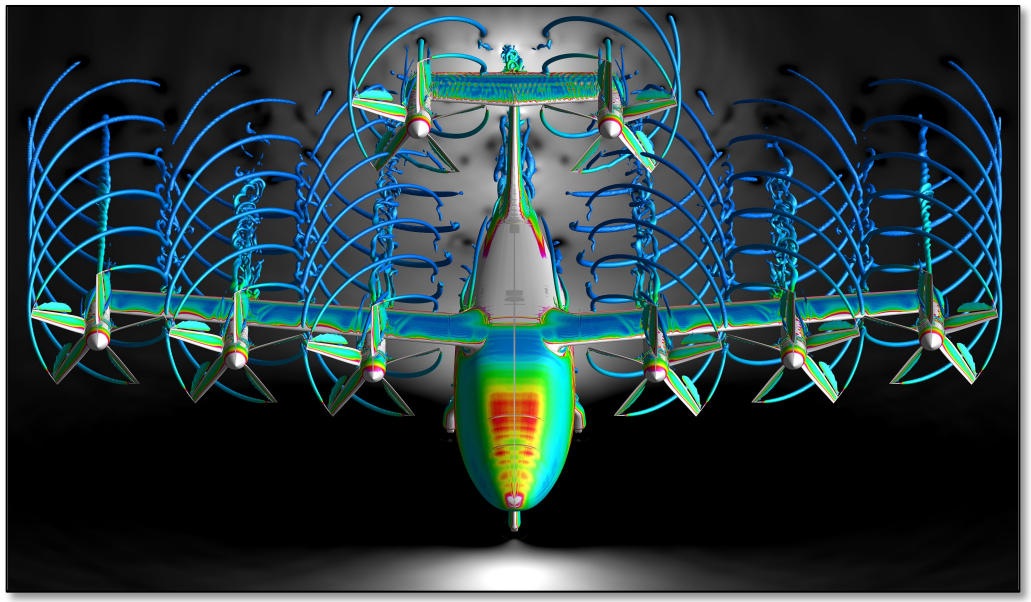
** HECC provided supercomputing resources and services in support of this work.*

Simulations for Designing Safe and Efficient Air Taxis*

- Utilizing HECC's Pleiades, Electra, and Aitken supercomputers, aerospace engineers at NASA Ames simulated the flow around different air taxi vehicle concepts. Understanding the complex flow structures in rotary-wing aircraft is key to designing quieter, safer, and more efficient Urban Air Mobility (UAM) vehicles.
- The engineers analyzed the performance of both the tiltwing and Quiet Single-Main Rotor (QSMR) helicopter concept vehicles. Results showed:
  - For the tiltwing configuration, an efficient cruise flight or "airplane-mode" can be achieved by tilting the wing back to a horizontal position.
  - For the QSMR configuration, drooping the tip and lowering the tip speed decreases the sound pressure level by 13 decibels when compared to the baseline rotor design. However, cruise performance is affected by these characteristics, and rotor lift-to-drag ratio drops by 60%.
- Over the past few years, the team has analyzed the performance of various NASA UAM concept vehicles. Different concepts, including a side-by-side rotorcraft and a quadcopter, have been simulated using high-fidelity computational fluid dynamics and HECC supercomputers.
- The simulations carried out on HECC supercomputers enabled the engineers to solve fine grids to capture the very fine details of the vortices and to accurately calculate UAM performance.

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

IMPACT: HECC's powerful supercomputers and mass storage systems are essential to solving these complex simulations in just a few days.



Visualization of the flow of NASA's six-passenger tiltwing concept for urban air mobility, in cruise or "airplane-mode" (front-oblique view). This image reveals the complexity of the flow for a tiltwing multi-rotor configuration, where many rotors interact with each other, the wing, and the fuselage. *Patricia Ventura Diaz and David Garcia, NASA Ames*

Papers

- "**Scattering of Ions at a Rippled Shock**," M. Gedalin, N. Pogorelov, V. Roytershetyn, *The Astrophysical Journal*, vol. 951, no. 1, published online July 4, 2023. *
  https://iopscience.iop.org/article/10.3847/1538-4357/acd63c/meta
- "**Effects of Full-Sphere Convection on M-Dwarf Dynamo Action, Flux Emergence, and Spin-Down**," C. Bice, J. Toomre, *The Astrophysical Journal*, vol. 951, no. 1, published online July 4, 2023. *
  https://iopscience.iop.org/article/10.3847/1538-4357/acd2db/meta
- "**Analysis of Exoplanet Detection Methods using Machine Learning and Deep Neural Networks**," J. Singh, N. Thoiba Singh, *IEEE Xplore*, presented at the 2023 International Conference on Sustainable Computing and Smart Systems, published online July 7, 2023. *
  https://ieeexplore.ieee.org/abstract/document/10169761
- "**Characteristics of Internal Tides from ECCO Salinity Estimates and Observations in the Bay of Bengal**," B. Subrahmanyam, V. Murty, S. Hall, *Remote Sensing*, vol. 15, issue 4 (Satellite-Based Sea Surface Salinity for Ocean Observation), July 10, 2023. *
  https://www.mdpi.com/2072-4292/15/14/3474
- "**Highly Accurate Potential Energy Surface and Dipole Moment Surface for Nitrous Oxide and 296K Infrared Line Lists for $^{14}N_2{}^{16}O$ and Minor Isotopologues**," X. Huang, D. Schwenke, T. Lee, *Molecular Physics* (Tim Lee Memorial Issue), July 11, 2023. *
  https://www.tandfonline.com/doi/full/10.1080/00268976.2023.2232892
- "**Dissipation and Time Step Scaling Strategies for Low and High Mach Number Flows**," S. Seraj, A. Yildirim, J. Anibal, J. Martins, *Journal of Computational Physics*, vol. 491, published online July 13, 2023. *
  https://www.sciencedirect.com/science/article/abs/pii/S0021999123004539

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

Papers (cont.)

- "**TOI 4201 b and TOI 5344 b: Discovery of Two Transiting Giant Planets around M-Dwarf Stars and Revised Parameters for Three Others**," J. Hartman, et al., arXiv:2307.06809 [astro-ph.EP], July 13, 2023. *
  https://arxiv.org/abs/2307.06809
- "**Halo Properties from Observable Measures of Environment: I. Halo and Subhalo Masses**," H. Bowden, P. Behroozi, A. Hearin, arXiv:2307.07549 [astro-ph.GA], July 14, 2023. *
  https://arxiv.org/abs/2307.07549
- "**Sources and Pathways of Glacier Meltwater in the Bellingshausen Sea, Antarctica**," P. Sheehan, et al., *Geophysical Research Letters*, vol. 50, issue 14, published online July 17, 2023. *
  https://agupubs.onlinelibrary.wiley.com/doi/full/10.1029/2023GL102785
- "**A Search for Stellar Siblings of the ~200 Myr TOI-251 b Planetary System**," Q. Sun, et al., *The Astrophysical Journal*, vol. 952, no. 1, published online July 18, 2023. *
  https://iopscience.iop.org/article/10.3847/1538-4357/acd346
- "**Discovery and Characterization of Two Neptune-mass Planets Orbiting HD 212729 with TESS**," D. Armstrong, et al., *Monthly Notices of the Royal Astronomical Society*, published online July 20, 2023. *
  https://academic.oup.com/mnras/advance-article/doi/10.1093/mnras/stad2183/7227347
- "**Non-Monotonic Feedback Dependence Under Abrupt CO2 Forcing Due to a North Atlantic Pattern Effect**," I. Mitevski, et al., *Geophysical Research Letters*, vol. 50, issue 14, published online July 24, 2023. *
  https://agupubs.onlinelibrary.wiley.com/doi/full/10.1029/2023GL103617

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Papers (cont.)

- "**Observations and Modeling of Unstable Proton and Alpha Particle Velocity Distributions in Sub-Alfenic Solar Wind at PSP Perihelia**," L. Ofman, et al., arXiv:2307.13410 [astro-ph.SR], July 25, 2023. *
  https://arxiv.org/abs/2307.13410
- "**The Photometric Variability of Massive Stars due to Gravity Waves Excited by Core Convection**," E. Anders, et al., *Nature Astronomy*, published online July 27, 2023. *
  https://www.nature.com/articles/s41550-023-02040-7
- "**An Unusually Low-Density Super-Earth Transiting the Bright Early-Type M-Dwarf GJ 1018 (TOI-244)**," A. Castro-González, et al., *Astronomy & Astrophysics*, vol. 675, July 2023. *
  https://www.aanda.org/articles/aa/full_html/2023/07/aa46550-23/aa46550-23.html

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Presentations

- "**Anisotropic Mach Cone Aligned Mesh Adaptation for Low Boom Simulations**," C. Ashby, J. Housman, J. Duensing, presented as part of the Advanced Modeling and Simulation seminar series, July 6, 2023.
  https://www.nas.nasa.gov/pubs/ams/2023/07-06-23.html
- "**Supercomputing in the Artemis Program**," D. Dalle, presented as part of the 2023 NASA Ames Summer Series, July 13, 2023.
- **TESS/Kepler Asteroseismic Science Consortium Workshop**, Honolulu, HI, July 15-21, 2023.
  - "**Modeling of Disk-Integrated Oscillations of Solar-Type Stars and the Stellar Jitter Effect**," I. Kitiashvili, A. Wray.
  - "**Asteroseismic Inversions of Mixed Acoustic-Gravity Modes Excitation in Main-Sequence Stars with Shallow Outer Convection**," A. Kosovichev, I. Kitiashvili.
  - "**3D Radiative Hydrodynamics Modeling of Acoustic and Gravity Modes Excitation in Main-Sequence Stars with Shallow Outer Convection**," I. Kitiashvili.
- "**Aerodynamic Shape Optimization of Heat Exchangers**," J. Anibal, presented as part of the Advanced Modeling and Simulation seminar series, July 20, 2023.
  https://www.nas.nasa.gov/pubs/ams/2023/07-20-23.html
- "**Chasing Shadows in the Night: How NASA's Kepler and TESS Missions are Revolutionizing Exoplanet Science**," J. Jenkins, presented as part of the 2023 NASA Ames Summer Series, July 25, 2023.
- "**Recent Enhancements to Modeling Sonic Boom Propagation using Augmented Burgers' Equation**," S. Rallabhandi, presented as part of the Advanced Modeling and Simulation seminar series, July 27, 2023.
  https://www.nas.nasa.gov/pubs/ams/2023/07-27-23.html

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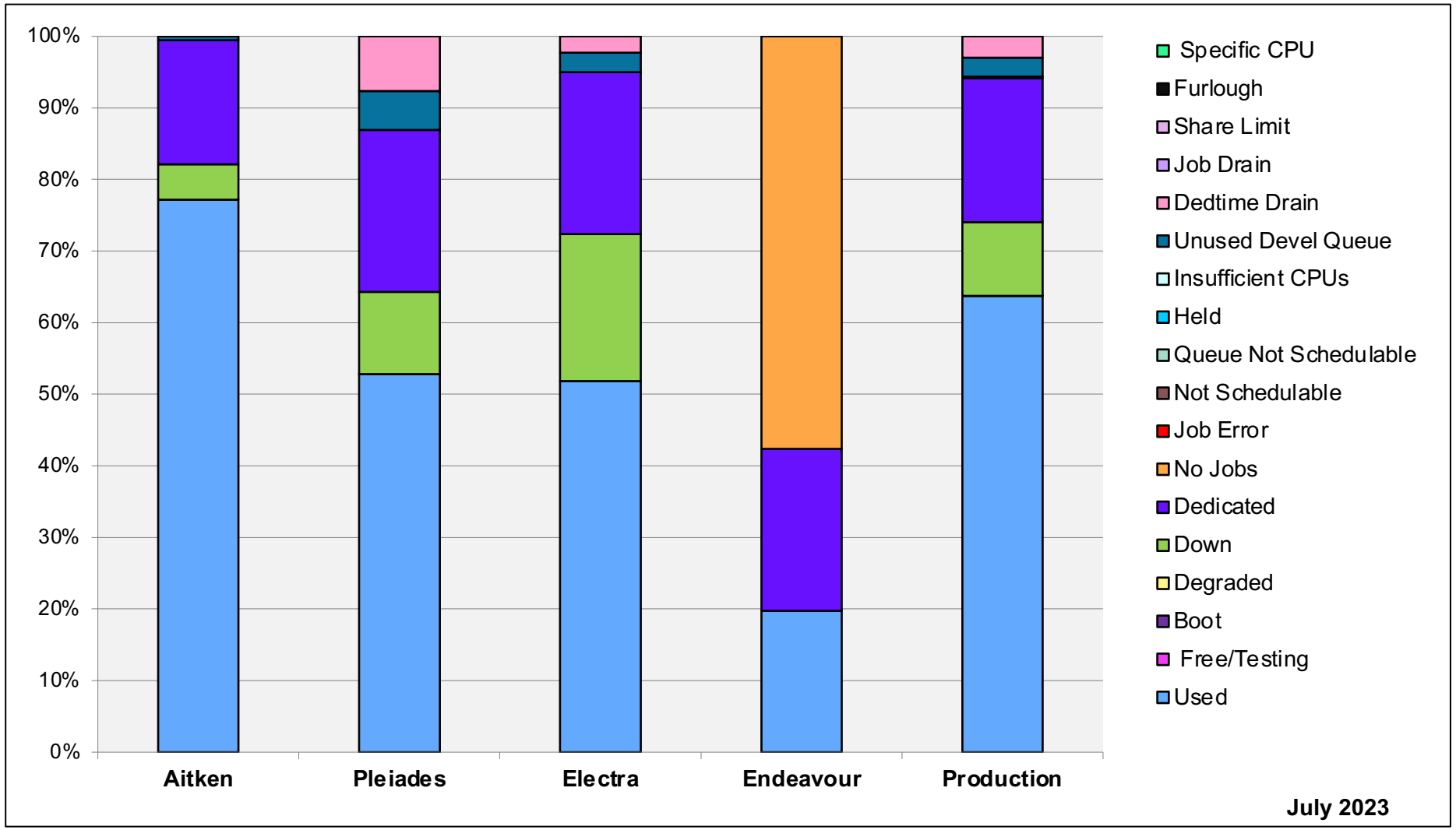
News and Events

- **APP Concierge Support for Hazardous Spring Forecast Experiment**, *HECC User Success Story*, July 18, 2023—Scientists in NASA's Global Modeling and Assimilation Office used the Aitken supercomputer to run their 2023 Hazardous Spring Forecast Experiment, which evaluates different ways to model severe weather over the continental U.S. Application optimization experts in the NAS Division provided extensive, customized "concierge service" throughout the three-month project to ensure its success. *https://www.nas.nasa.gov/hecc/about/hecc_user_success.html#APP_forecast*

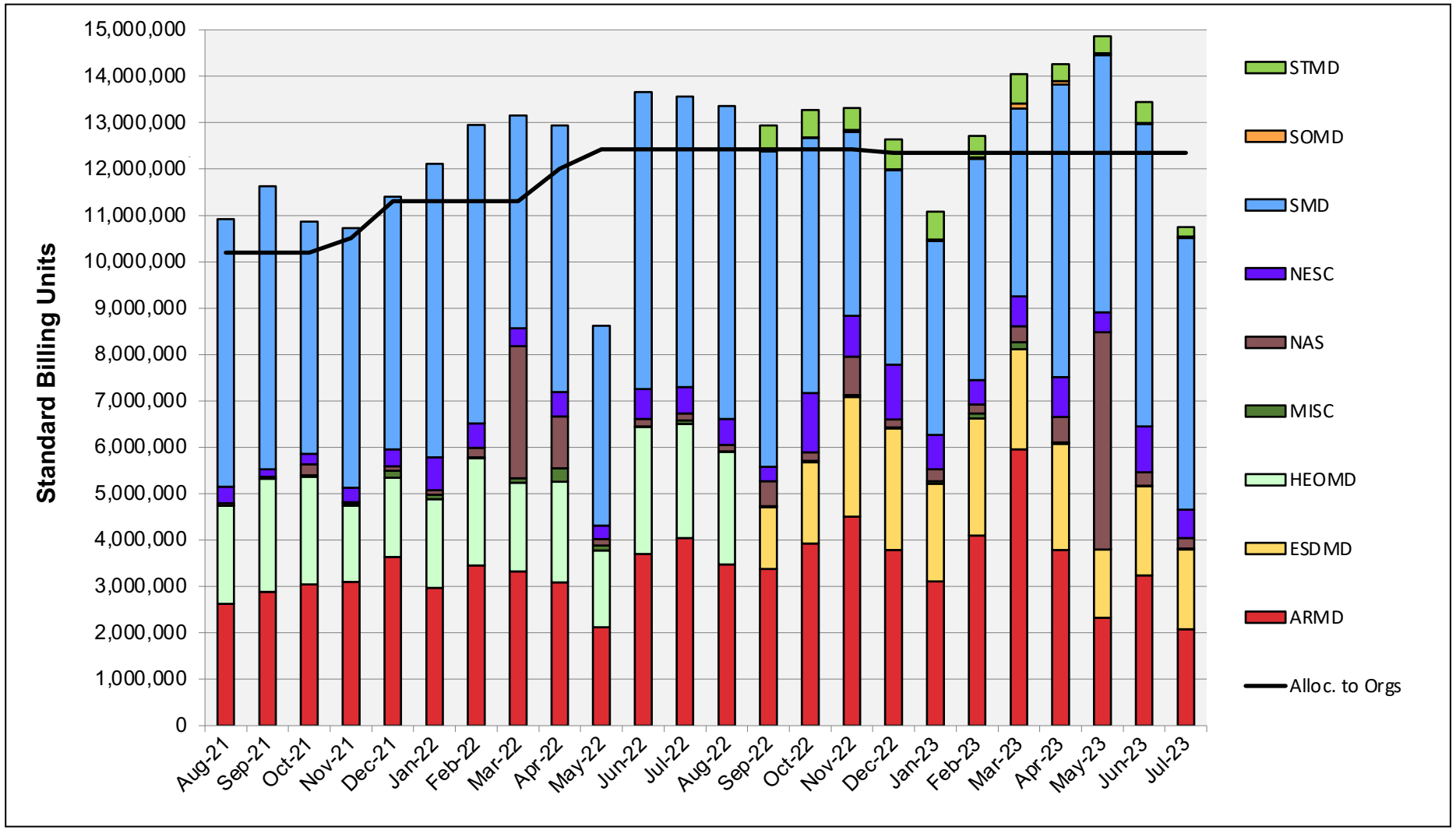
News and Events: Social Media

- **2023 Ames Summer Series Presentations**
  - NASA's Use of Supercomputing in the Artemis Program (Derek Dalle)
    - NAS: Twitter 7 retweets, 16 likes, ~1,029 impressions.
  - Chasing Shadows in the Night: How NASA's Kepler and TESS Missions are Revolutionizing Exoplanet Science (Jon Jenkins)
    - NAS: Twitter 4 retweets, 7 likes, ~723 impressions.

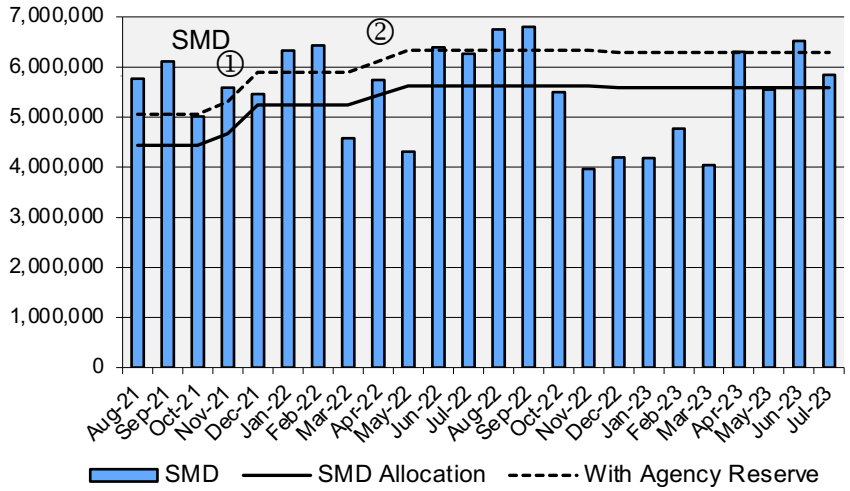
HECC Utilization

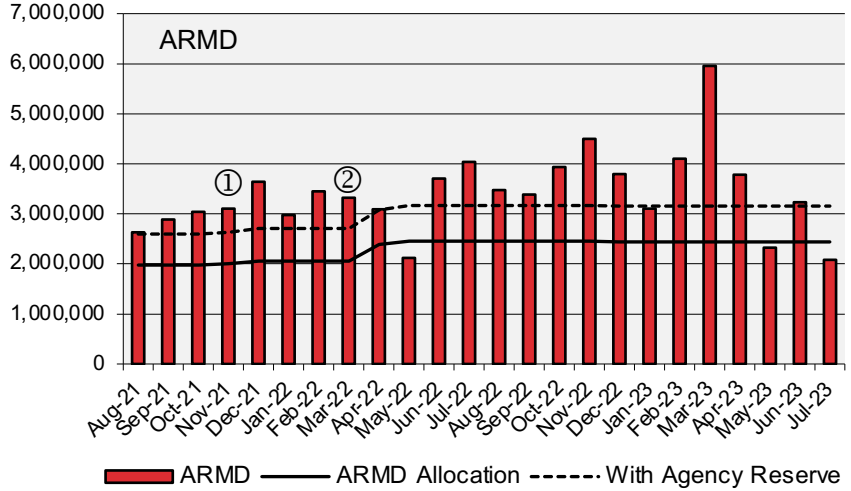


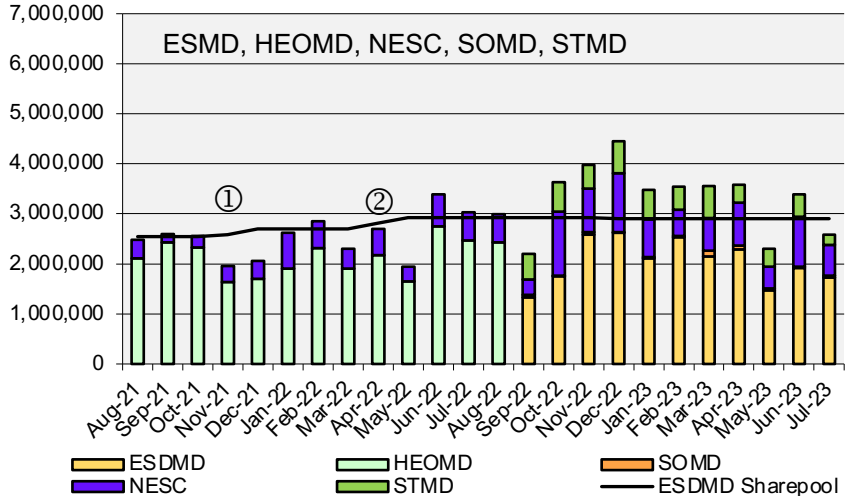
HECC Utilization Normalized to 30-Day Month



HECC Utilization Normalized to 30-Day Month



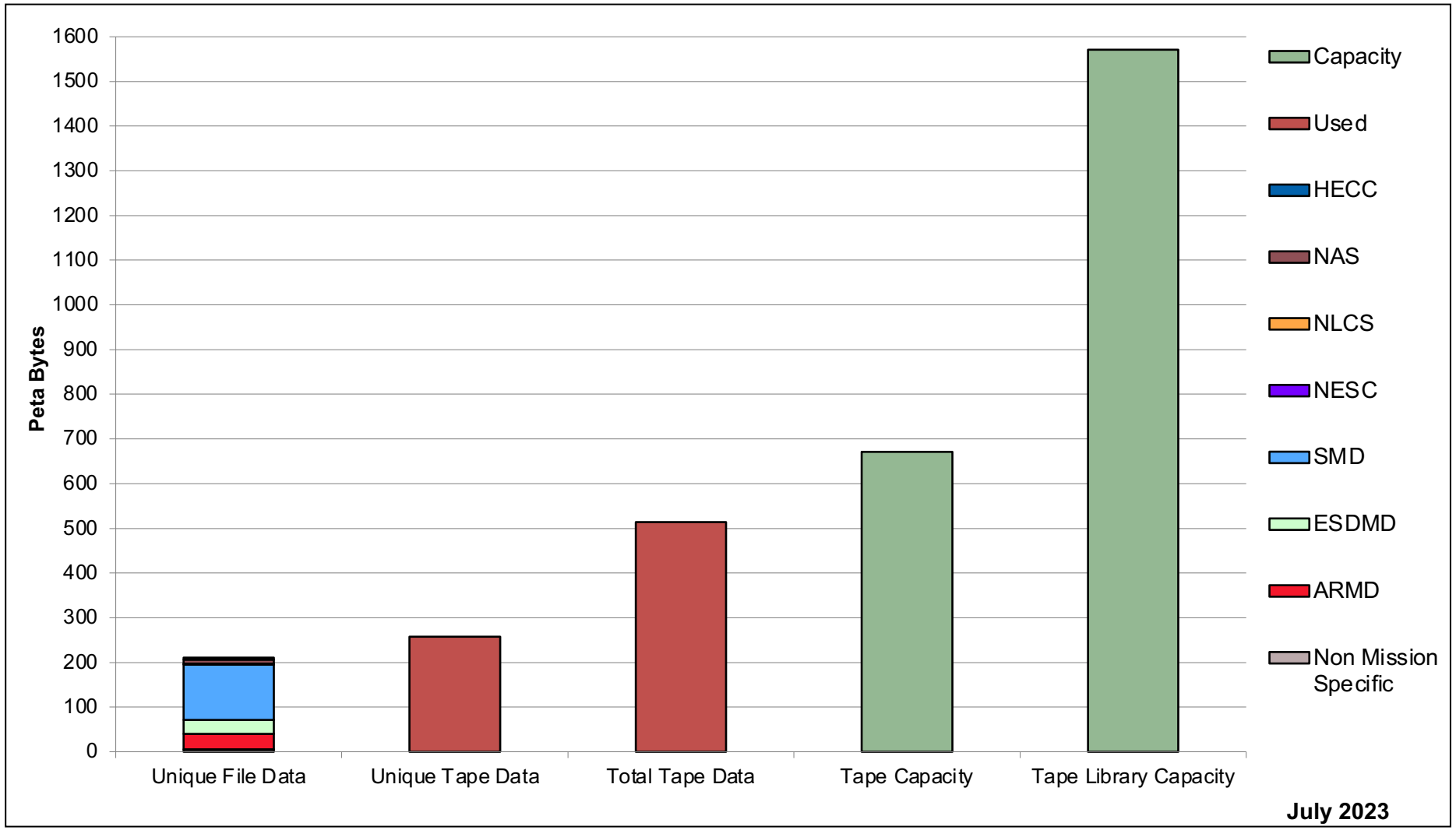




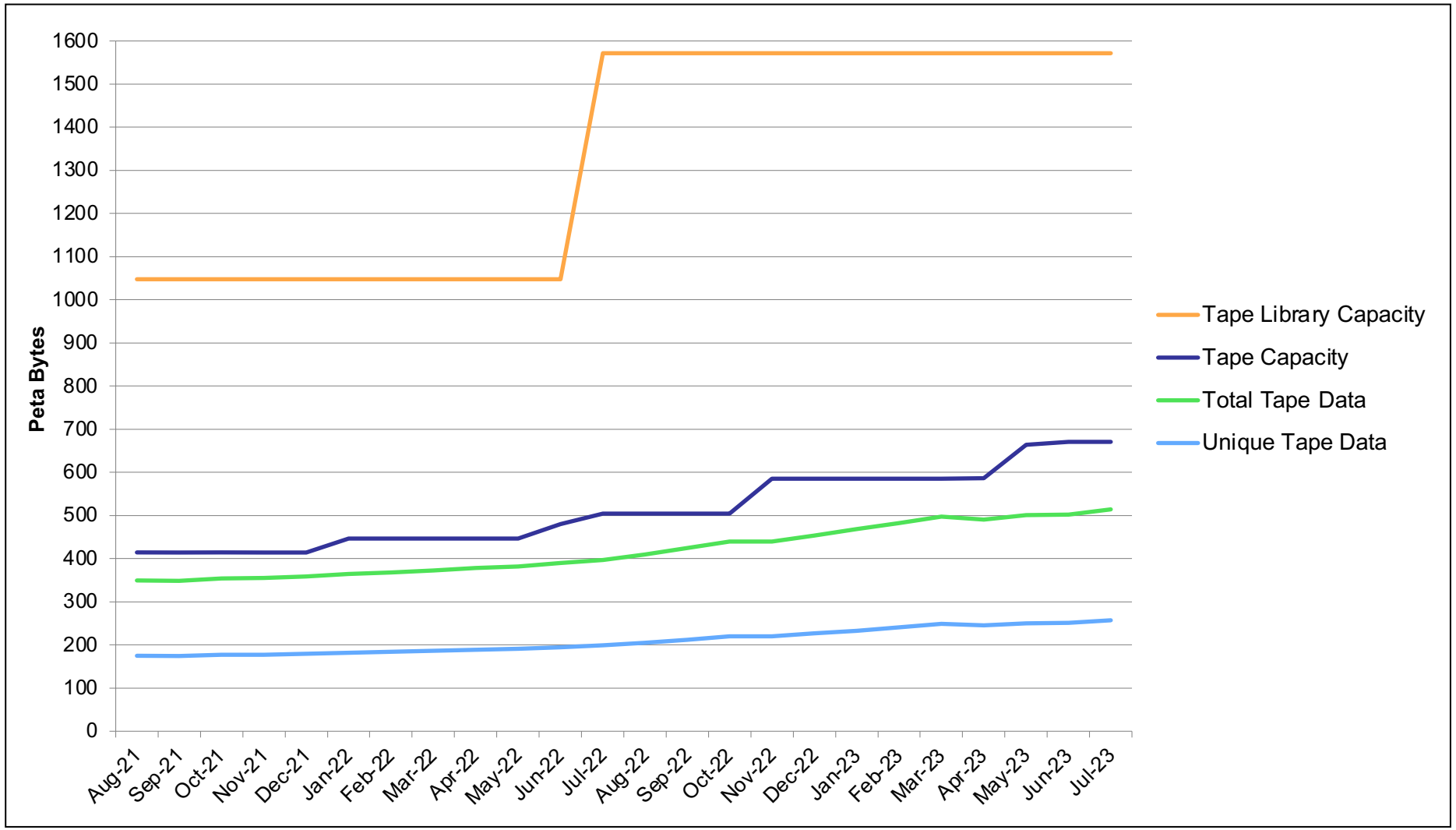
① 4 Rome Apollo Racks added to Aitken

② 4 Rome Apollo Racks added to Aitken

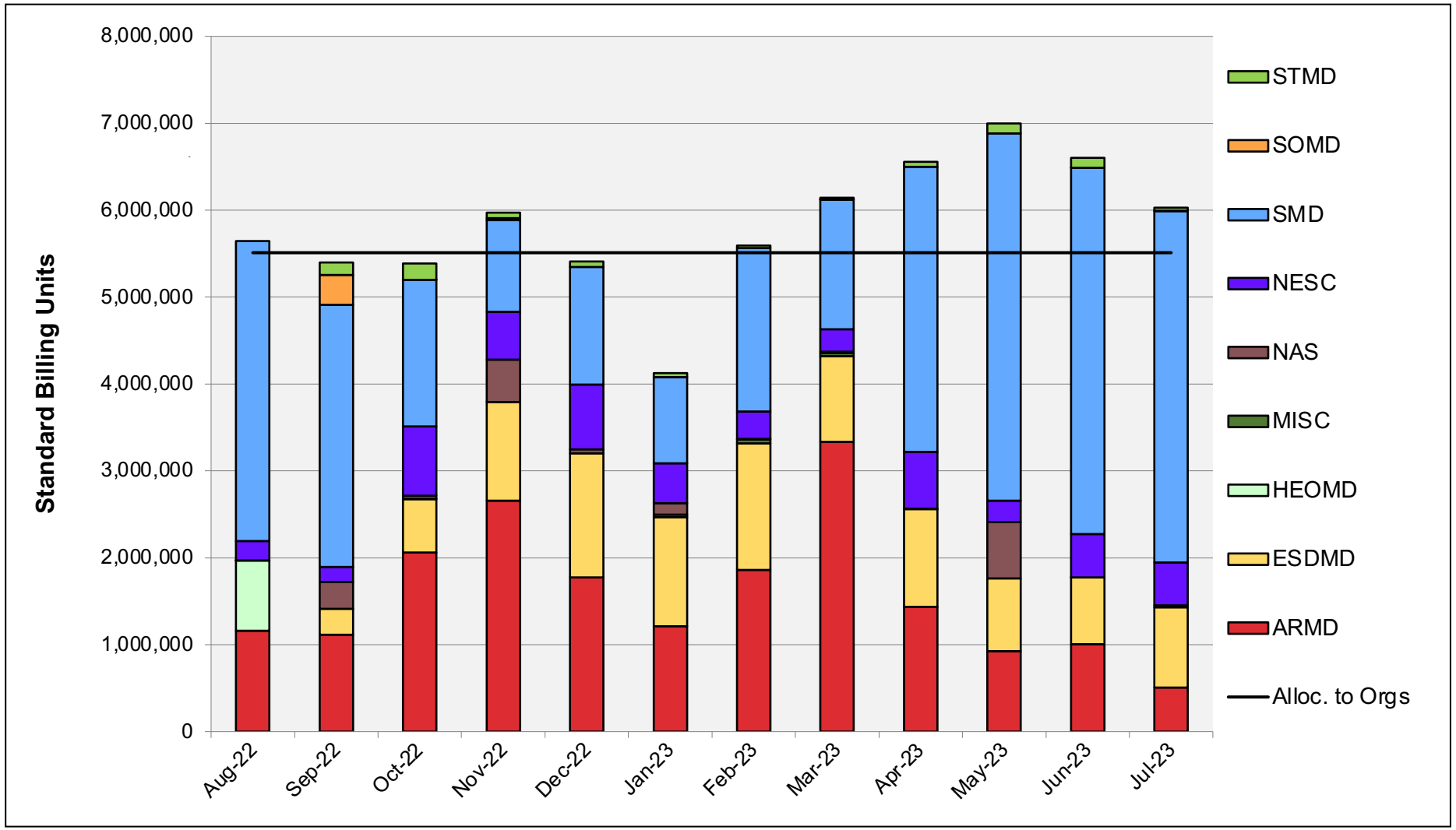
Tape Archive Status



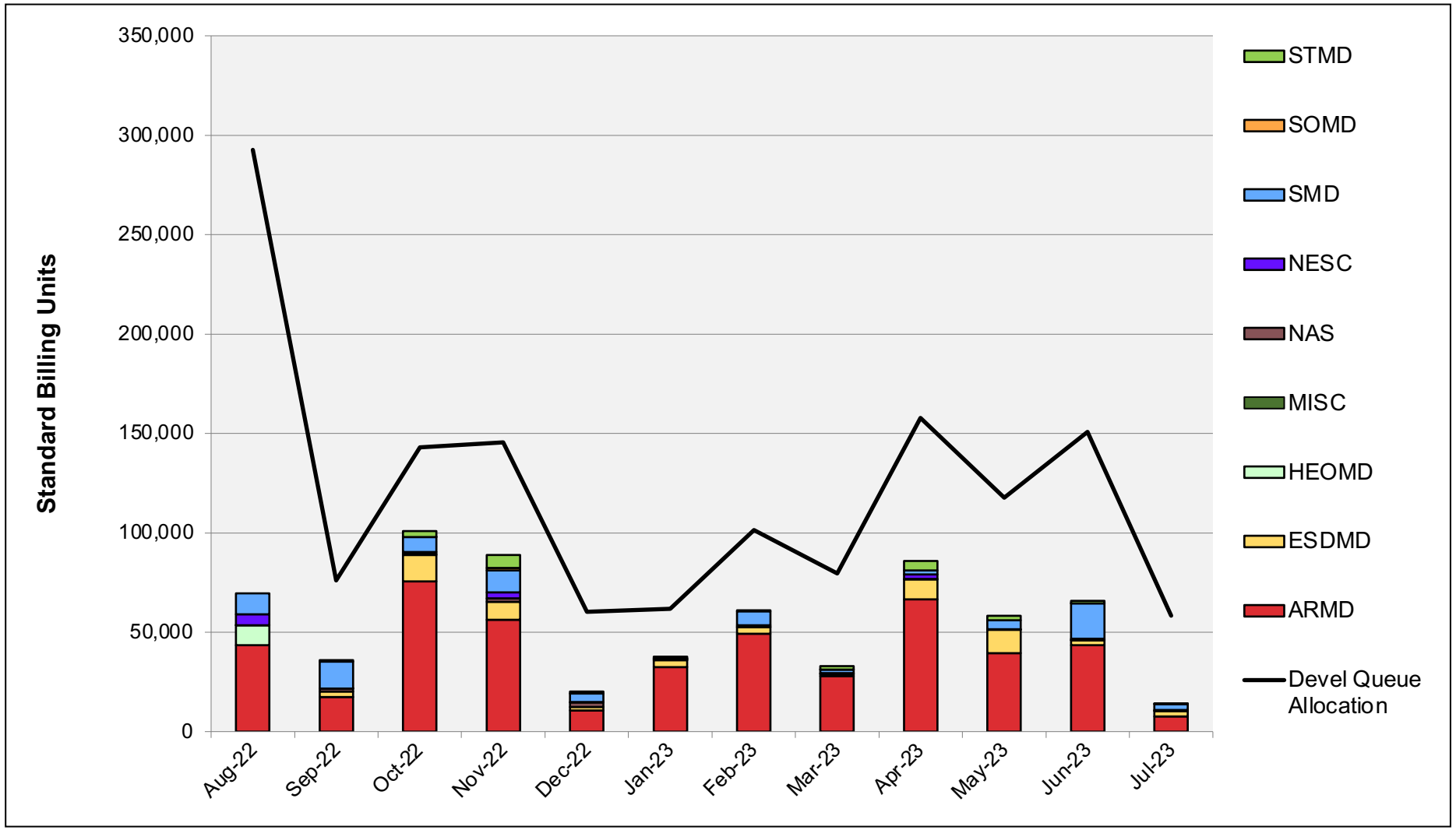
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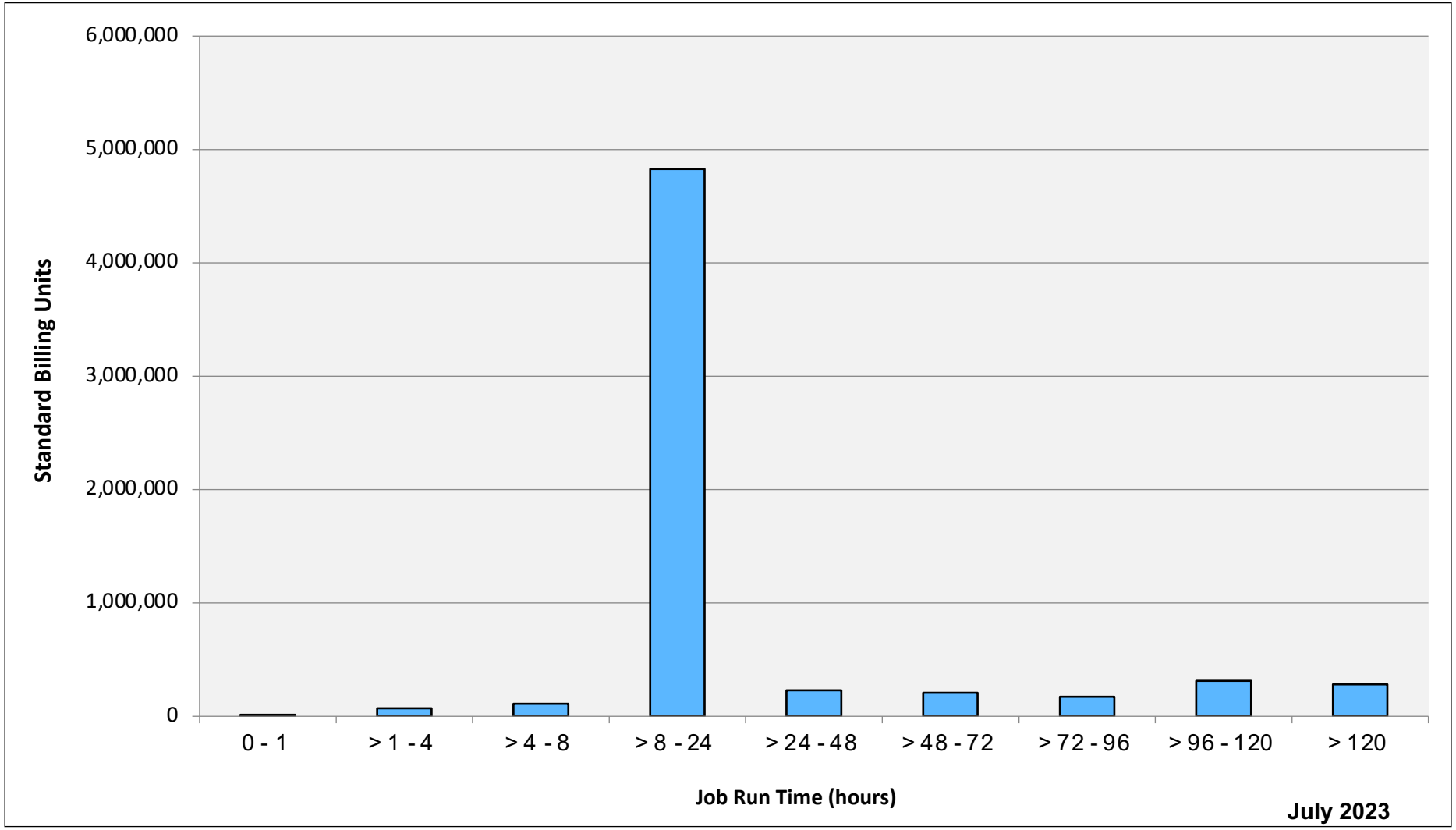
Aitken: SBUs Reported, Normalized to 30-Day Month



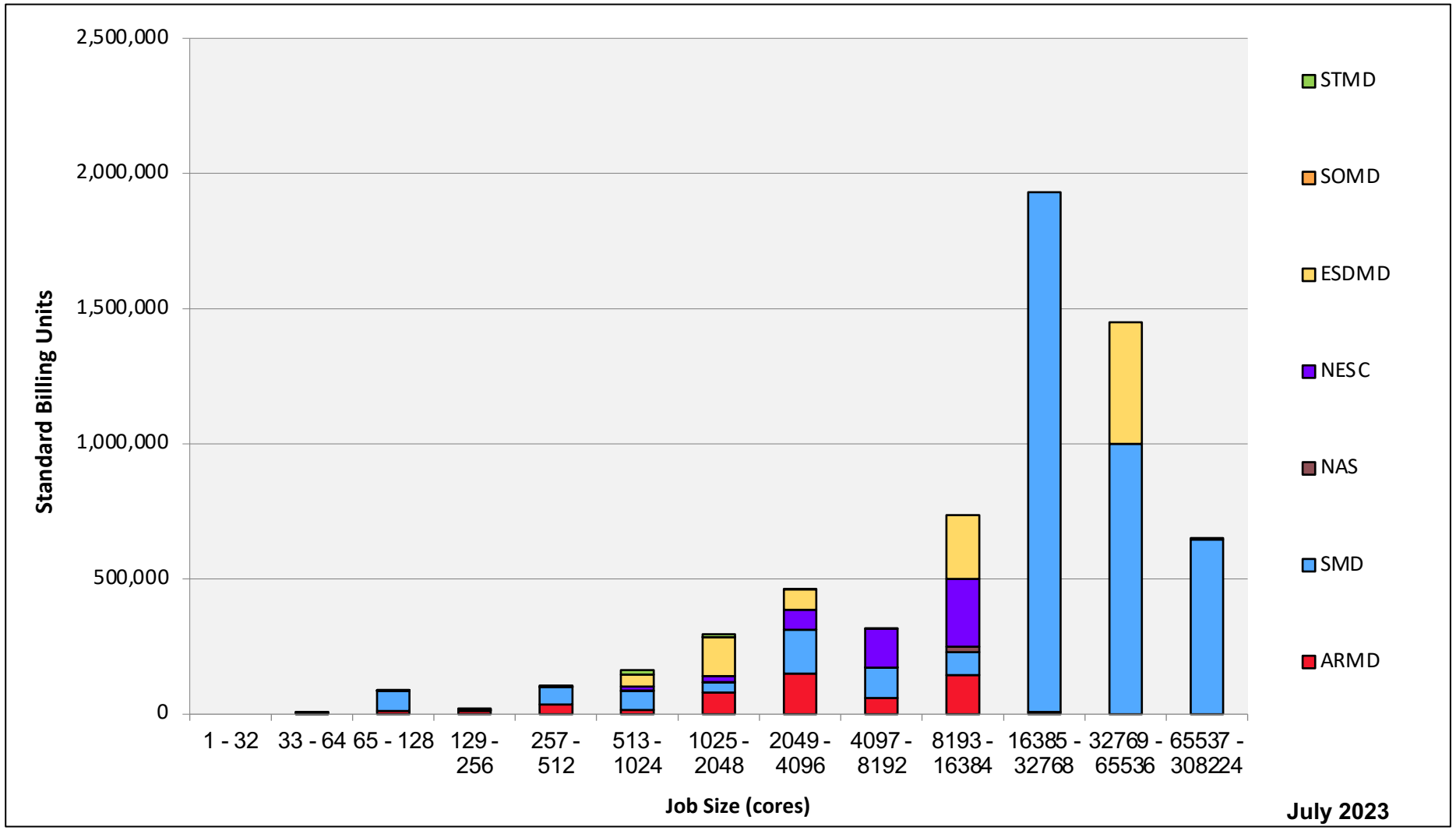
Aitken: Devel Queue Utilization



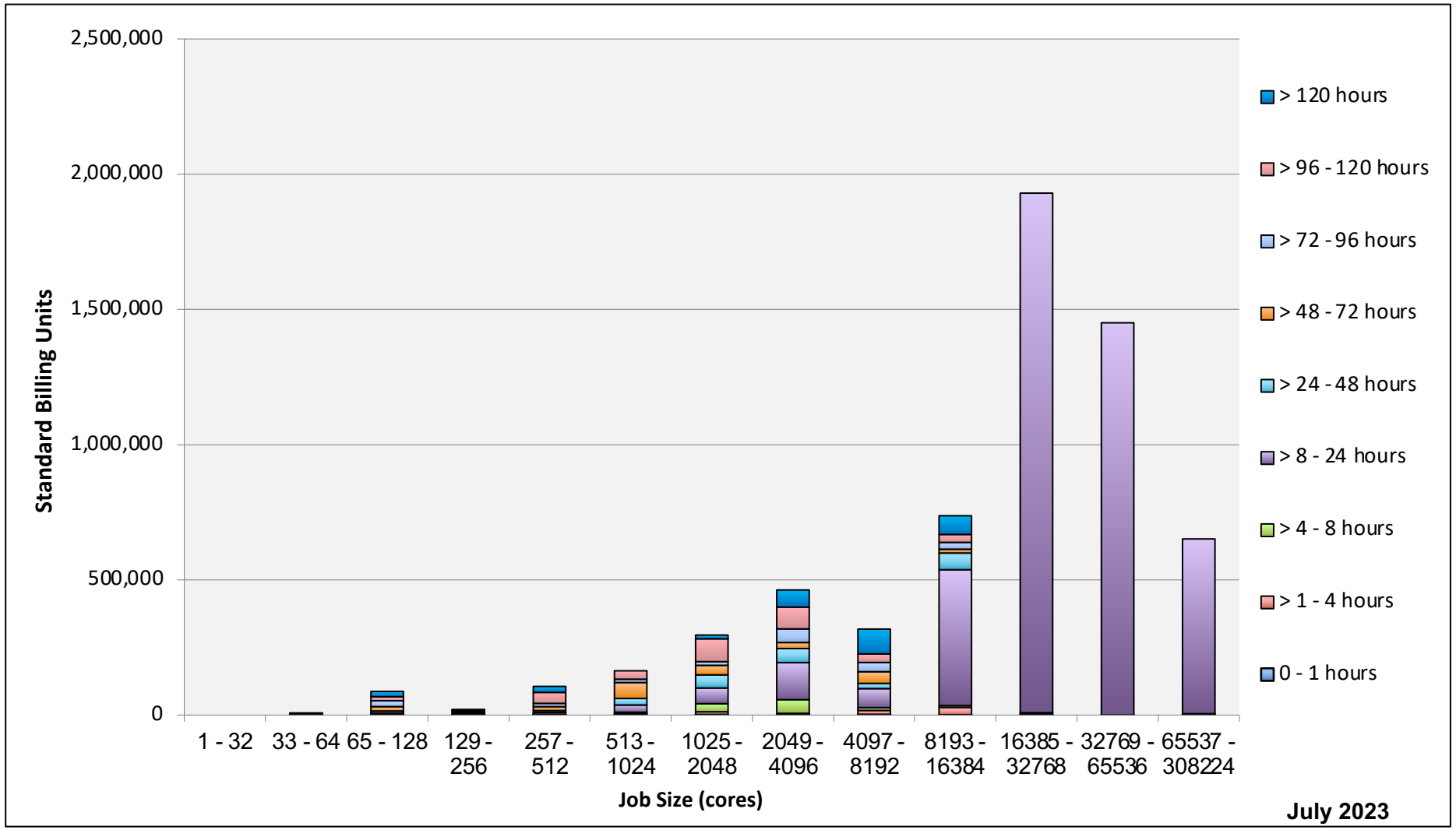
Aitken: Monthly Utilization by Job Length



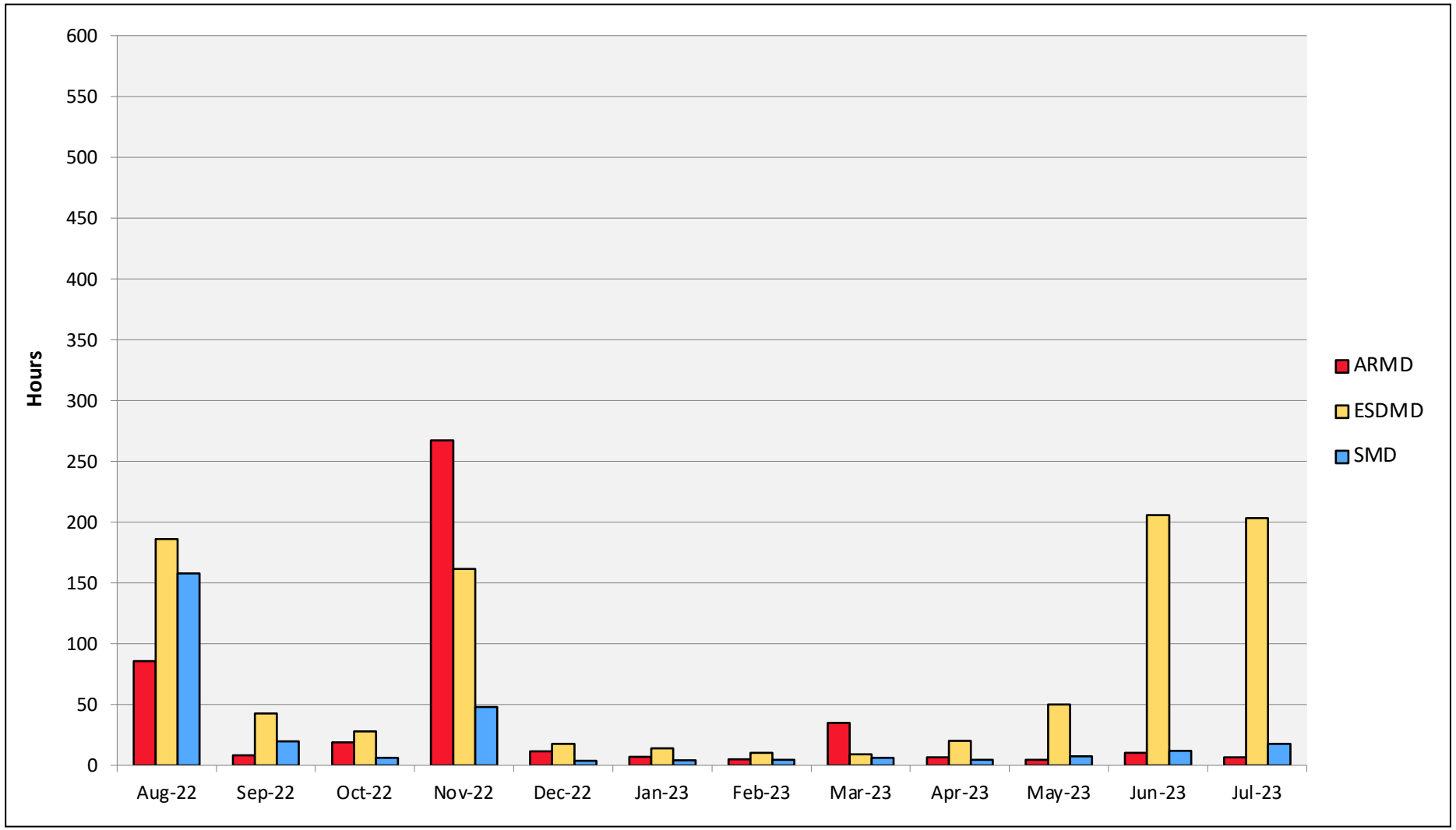
Aitken: Monthly Utilization by Job Size



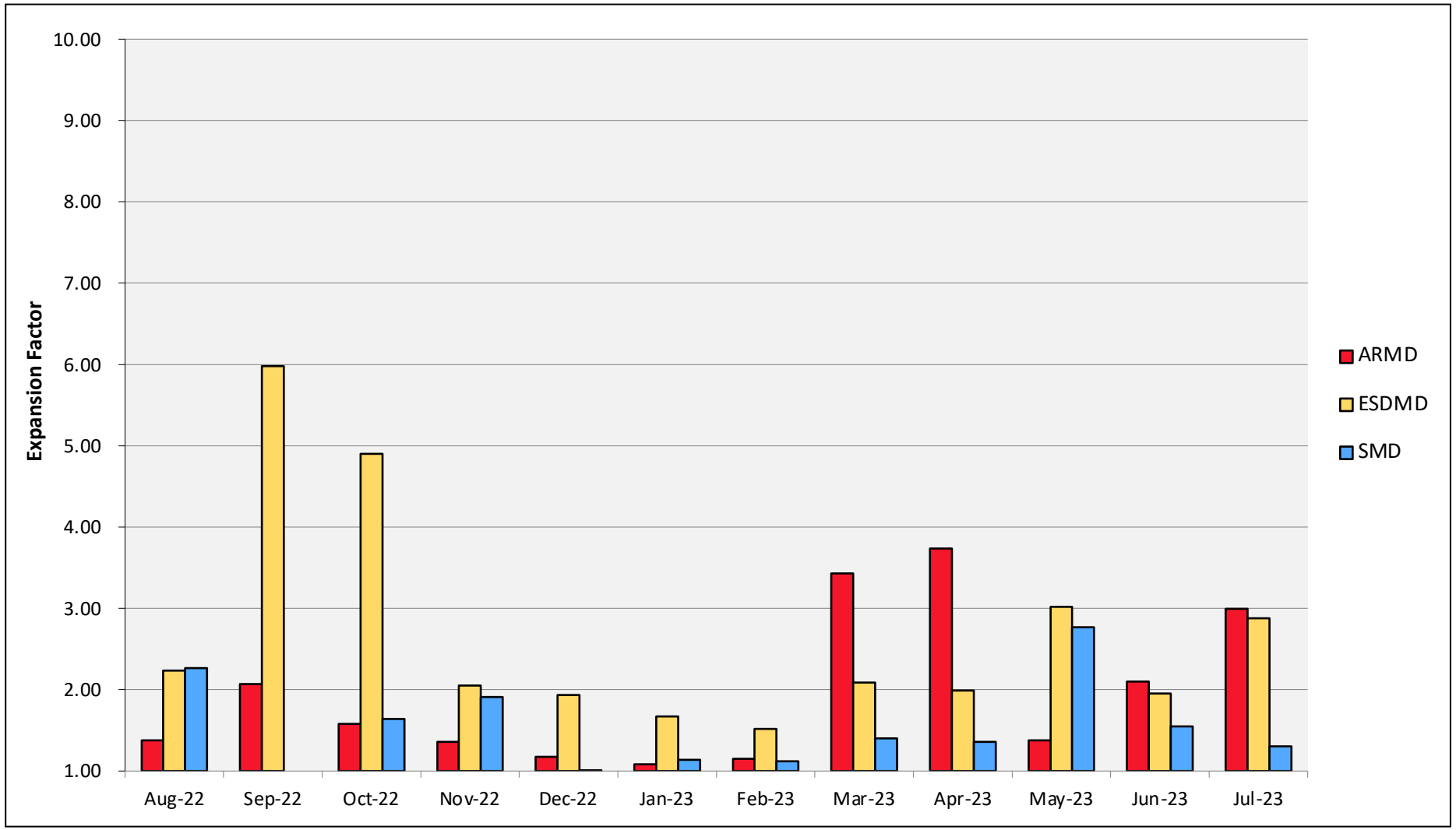
Aitken: Monthly Utilization by Size and Length



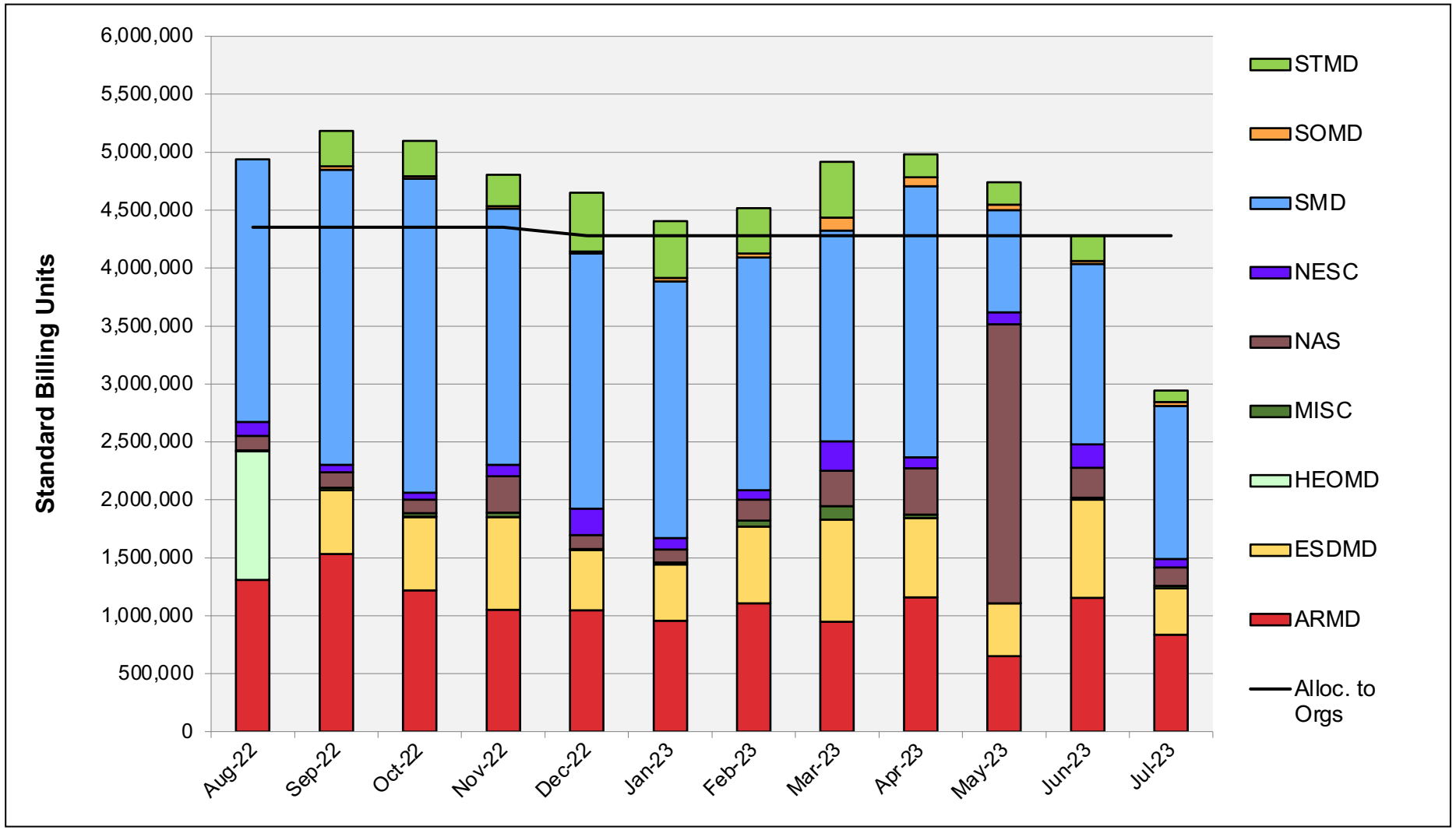
Aitken: Average Time to Clear All Jobs



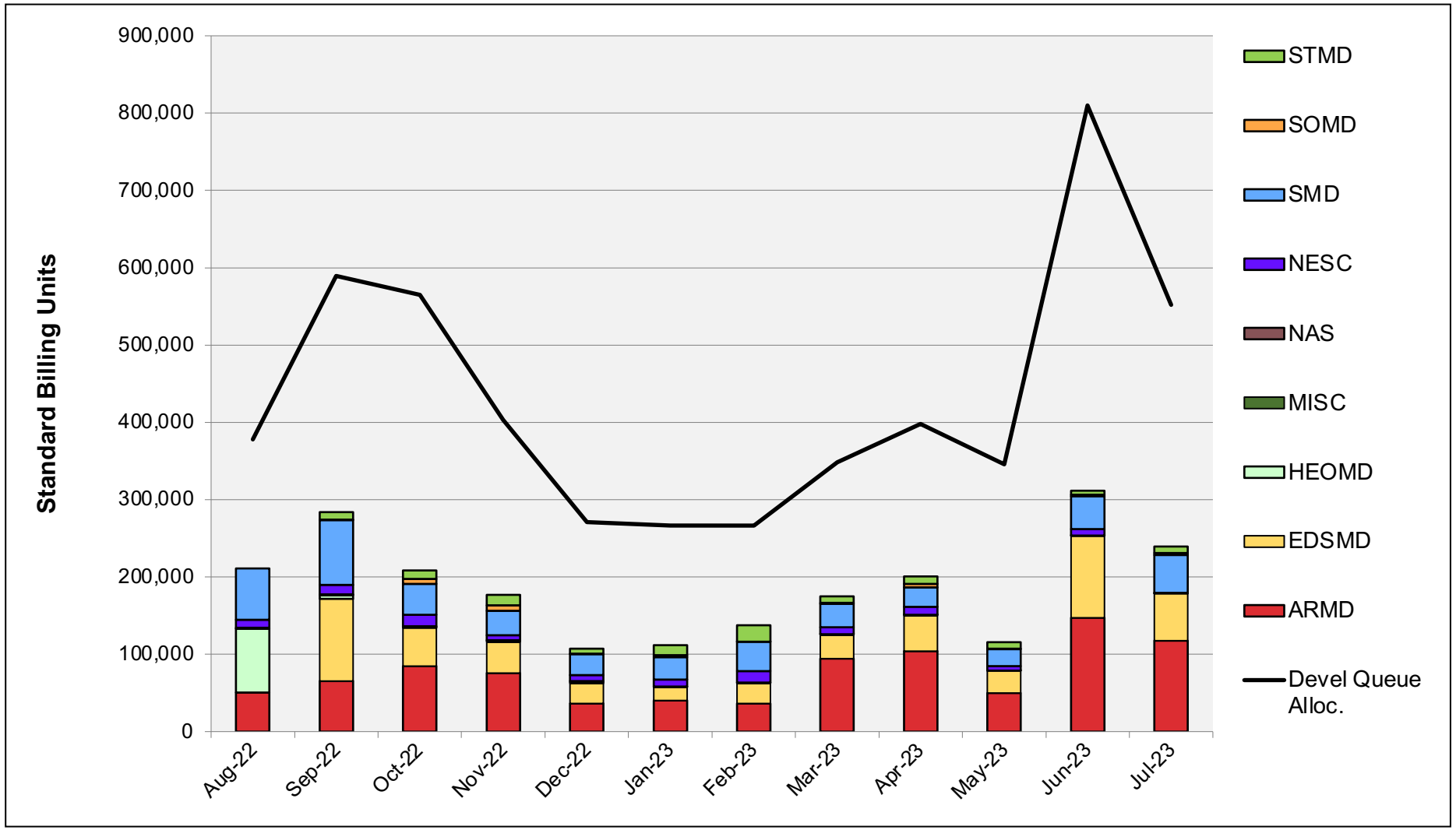
Aitken: Average Expansion Factor



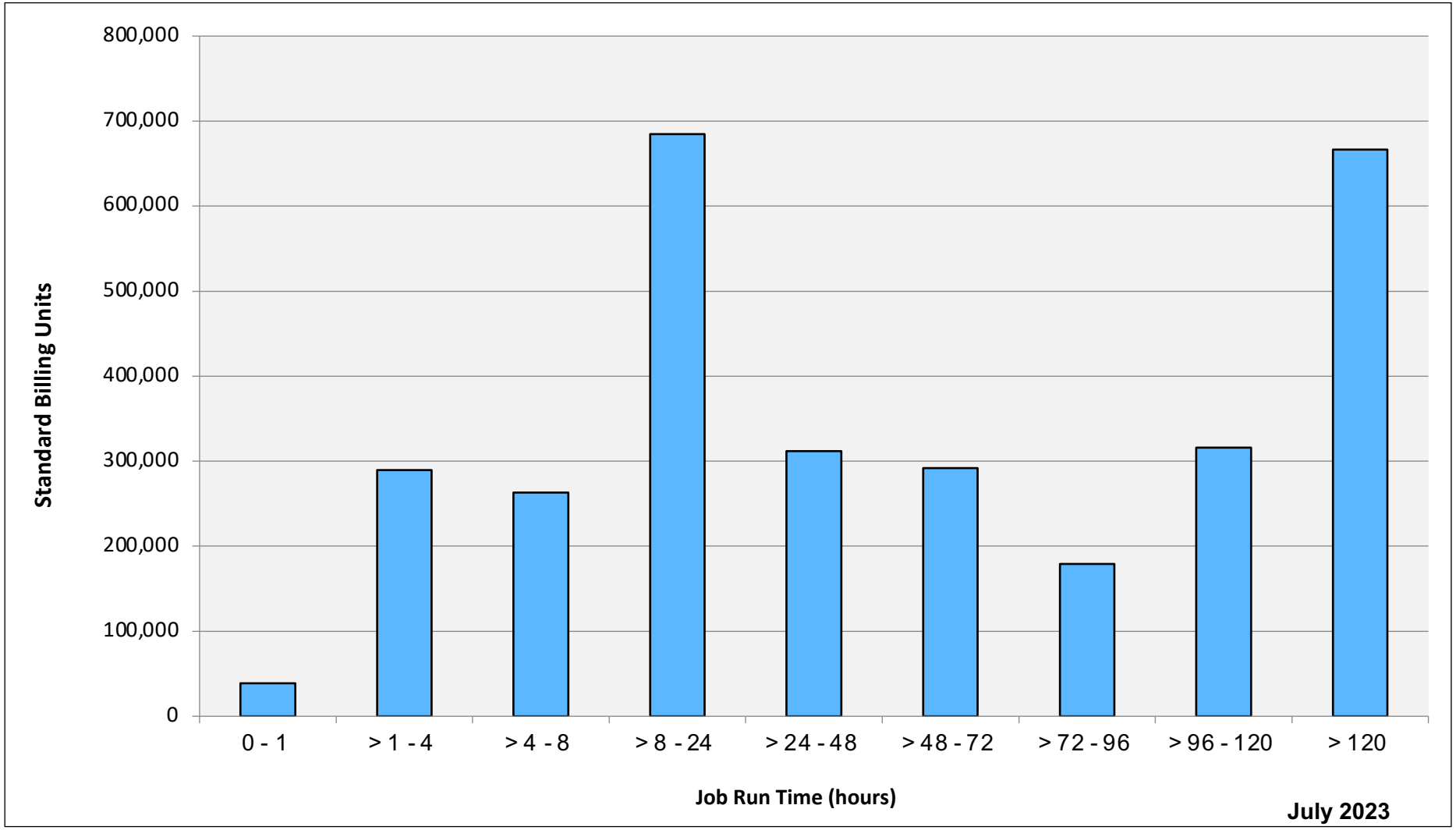
Pleiades: SBUs Reported, Normalized to 30-Day Month



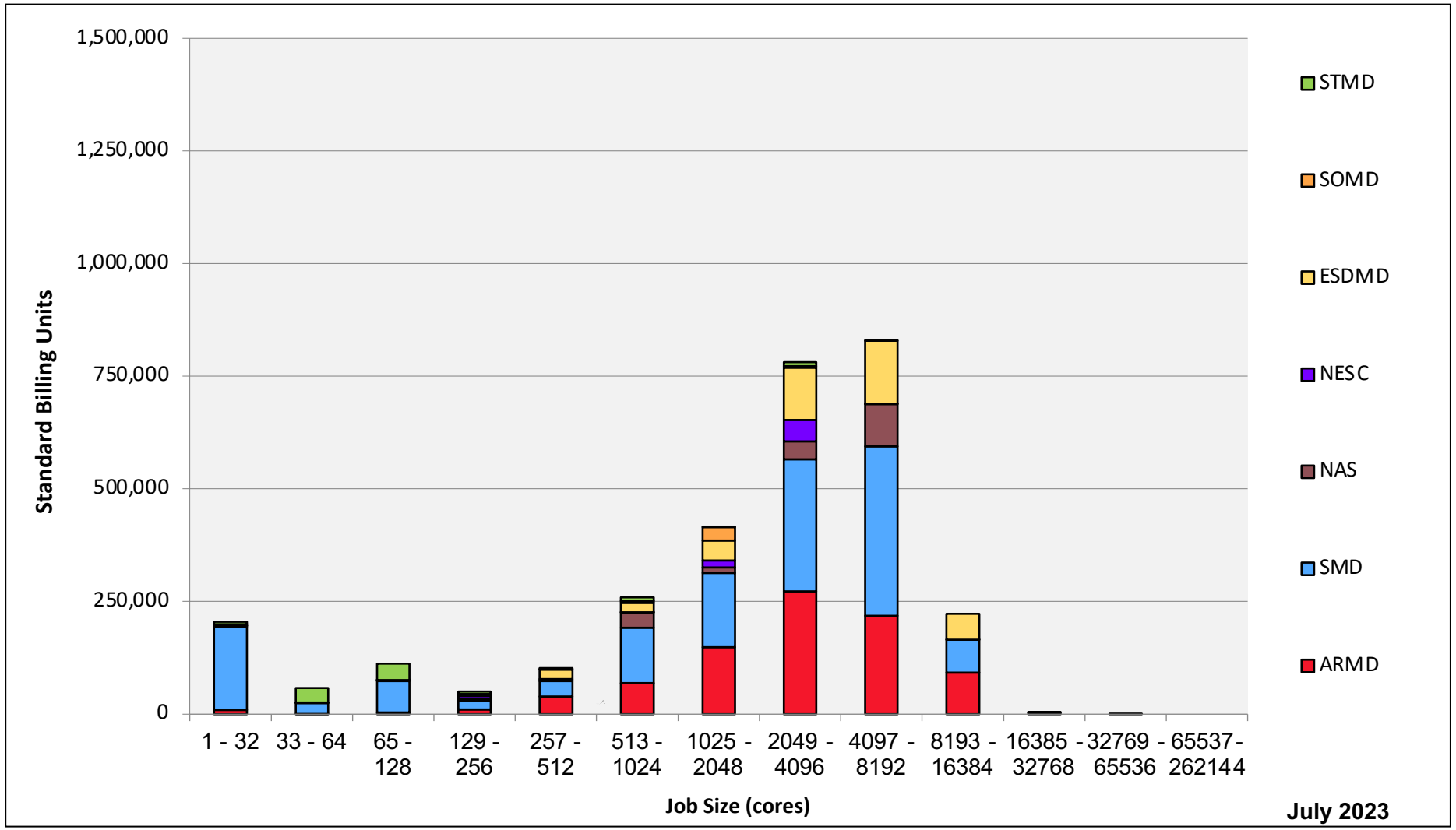
Pleiades: Devel Queue Utilization



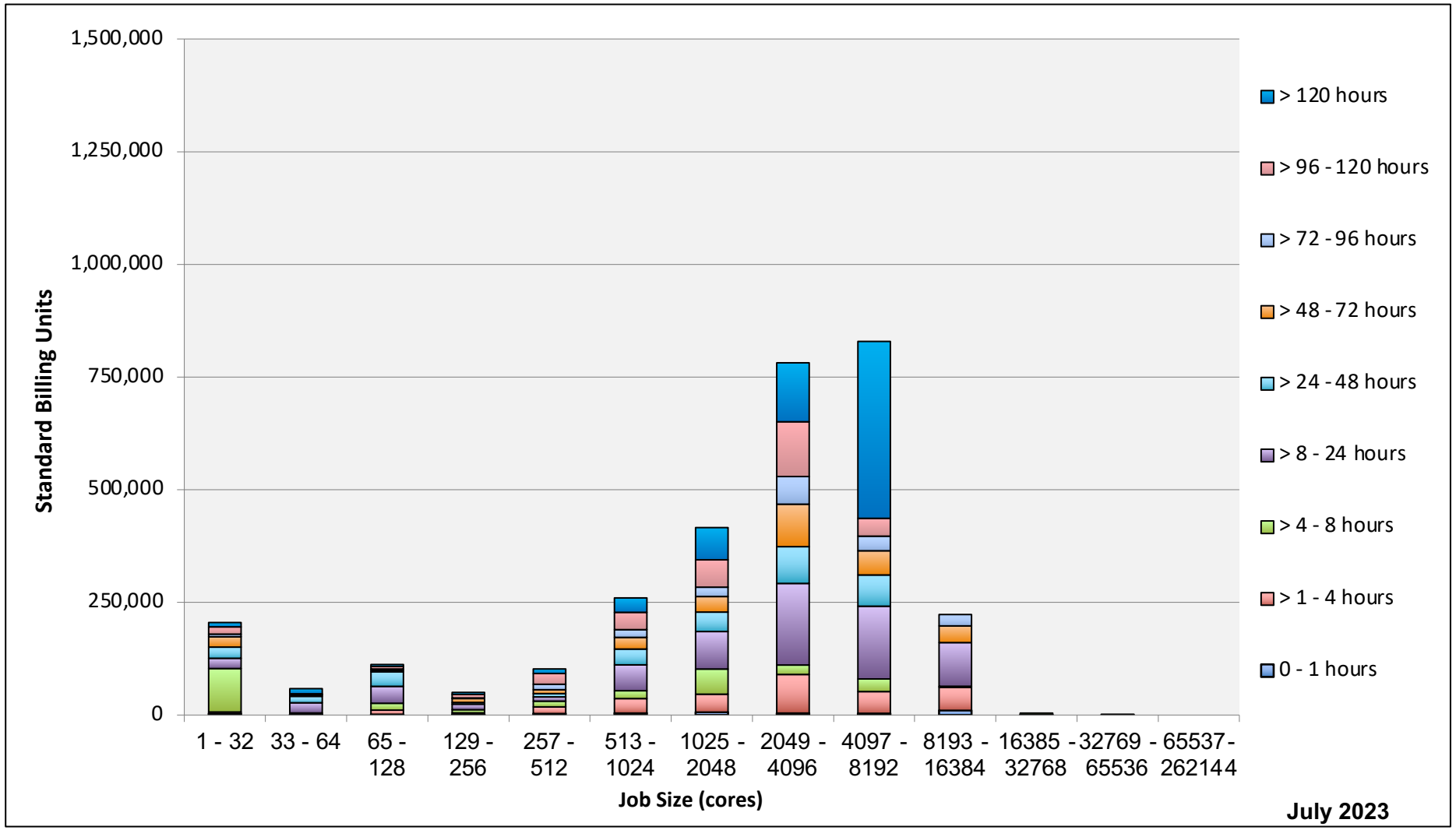
Pleiades: Monthly Utilization by Job Length



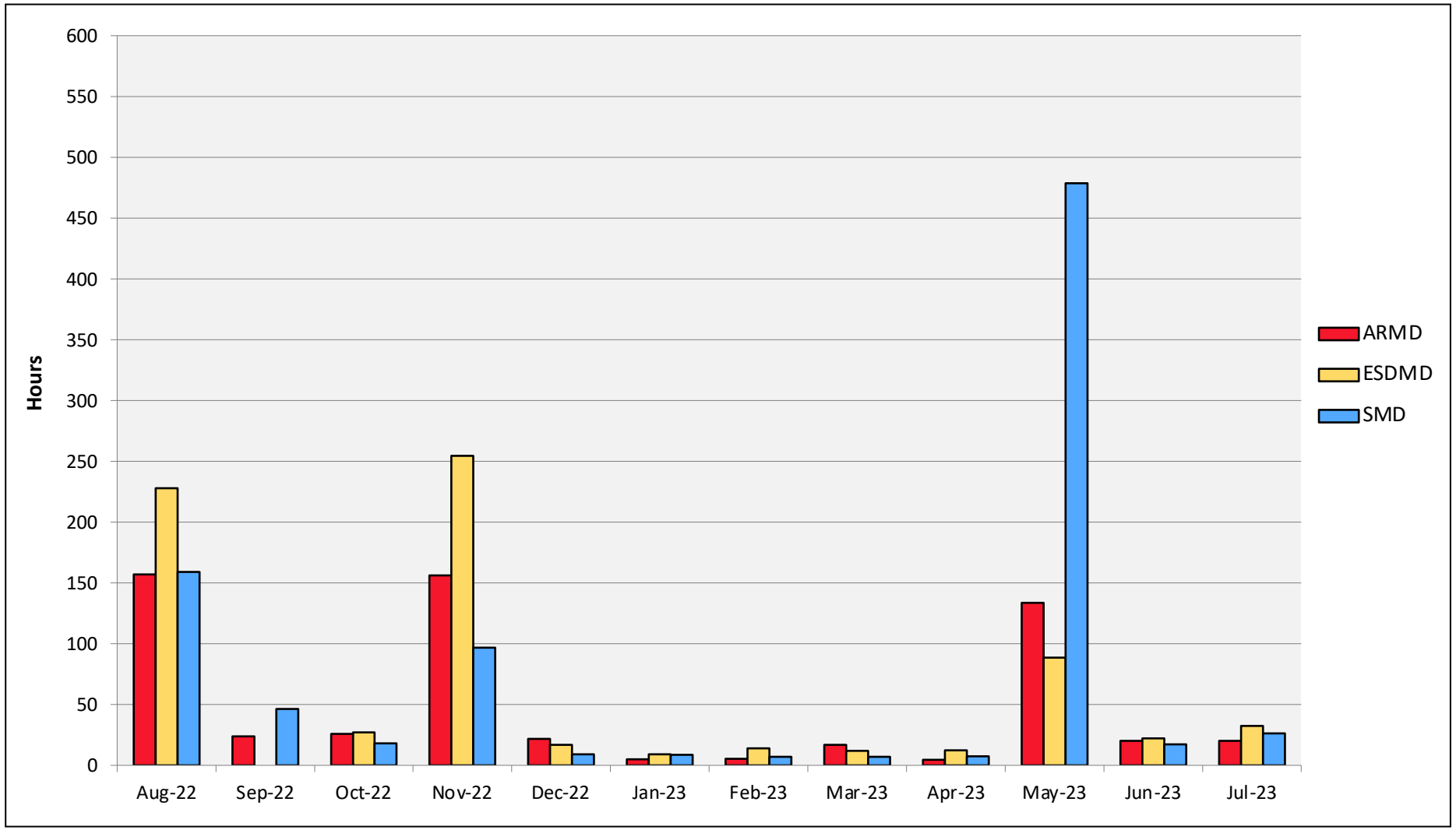
Pleiades: Monthly Utilization by Job Size



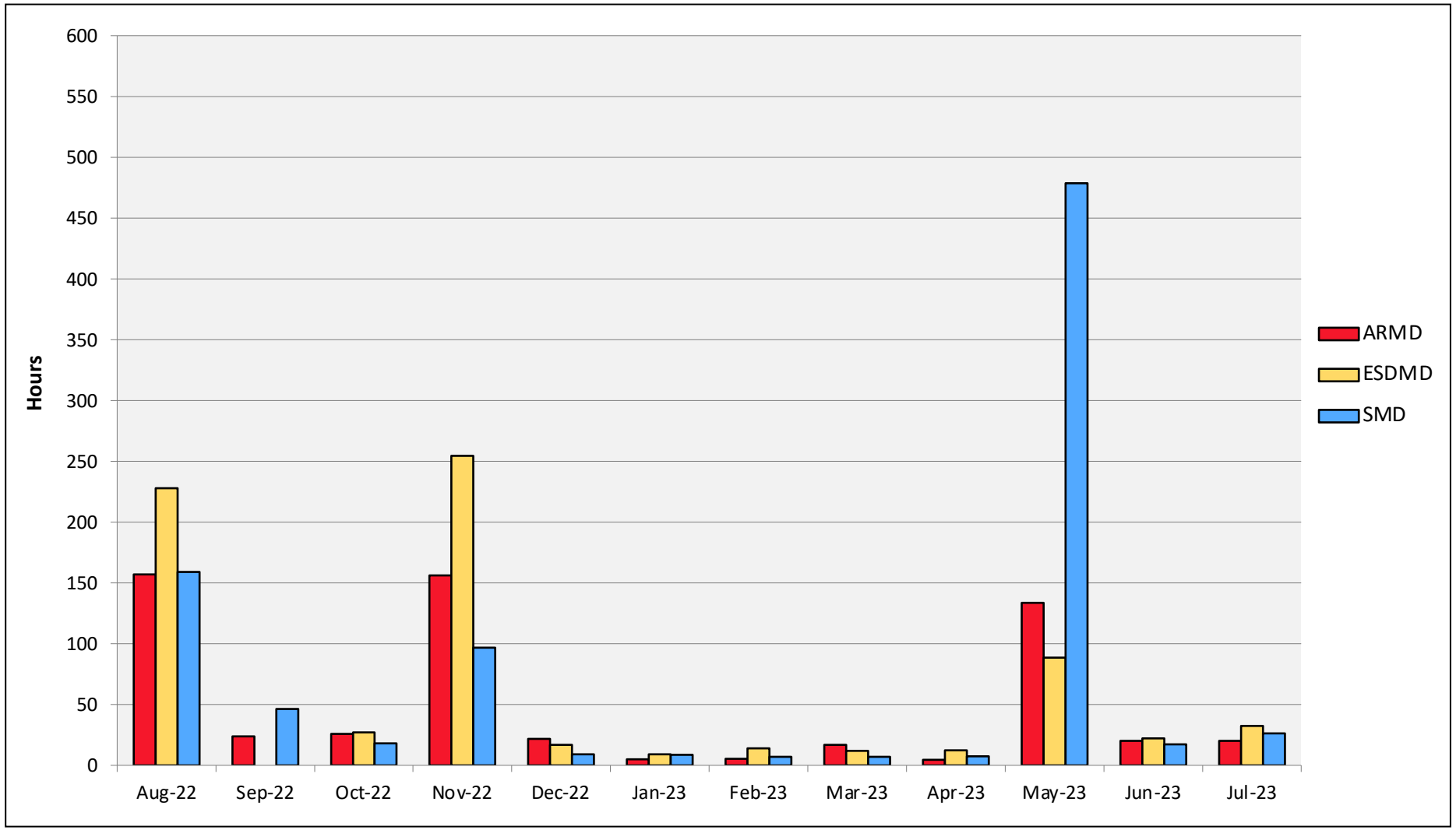
Pleiades: Monthly Utilization by Size and Length



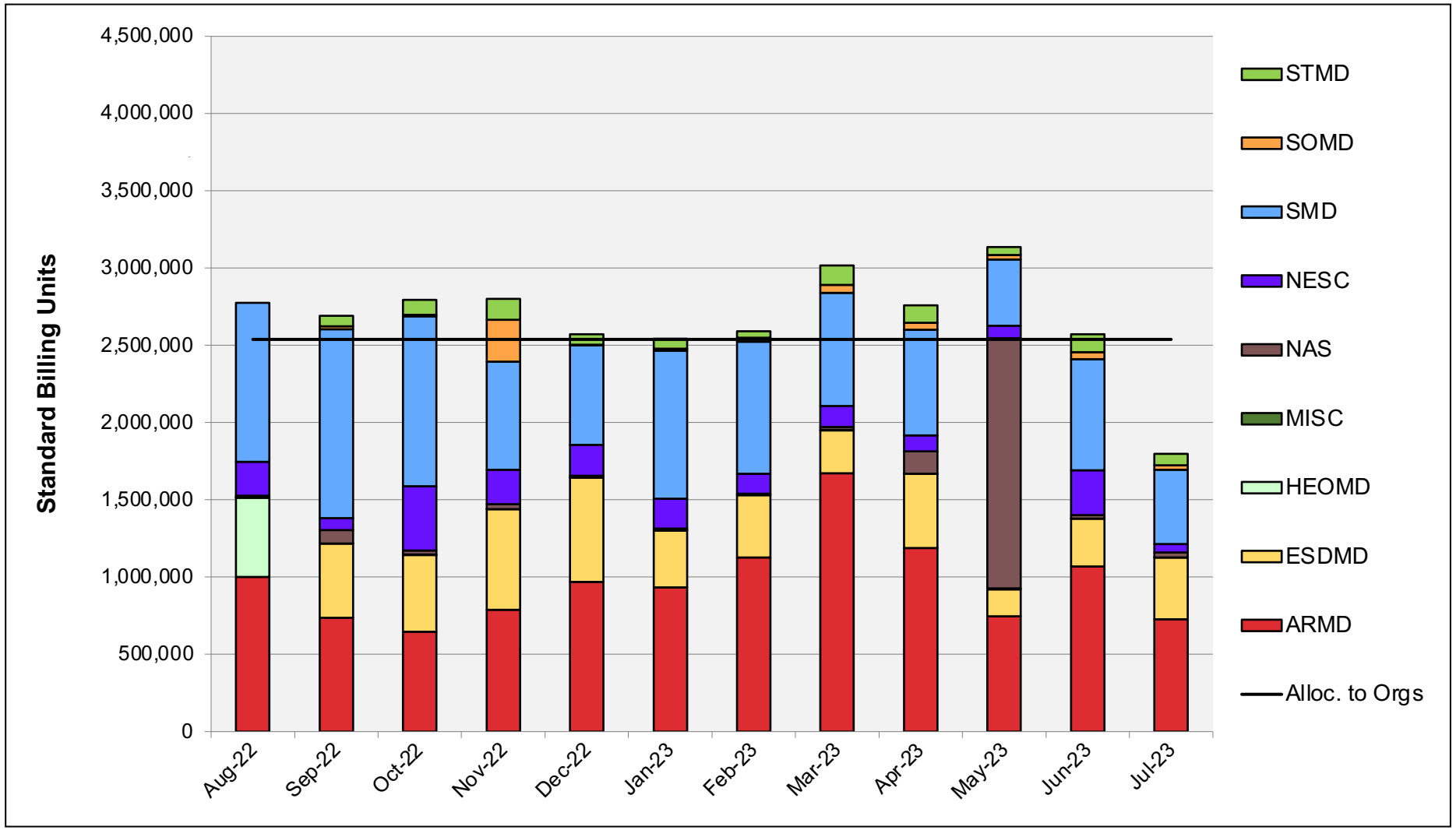
Pleiades: Average Time to Clear All Jobs



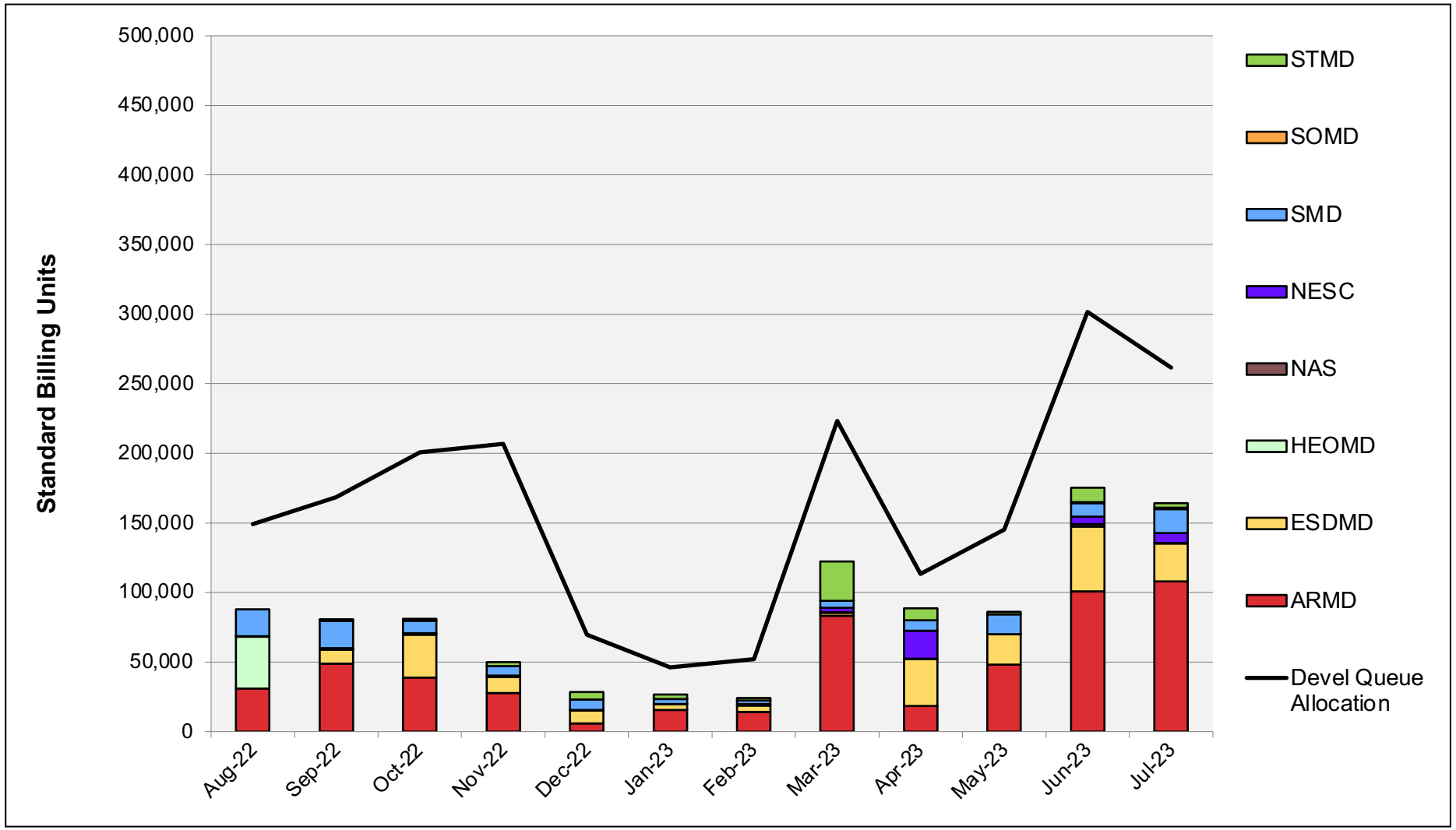
Pleiades: Average Expansion Factor



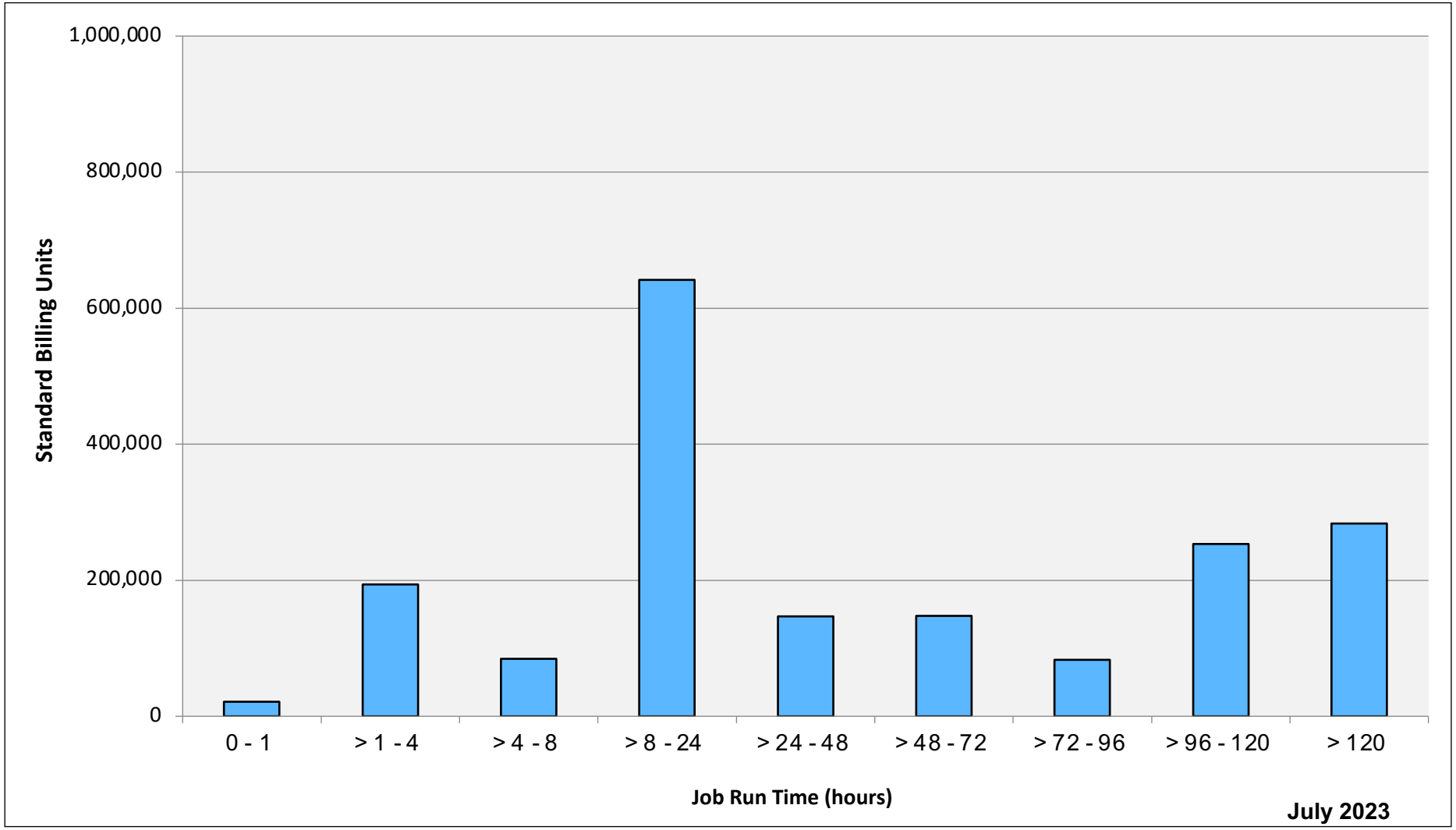
Electra: SBUs Reported, Normalized to 30-Day Month



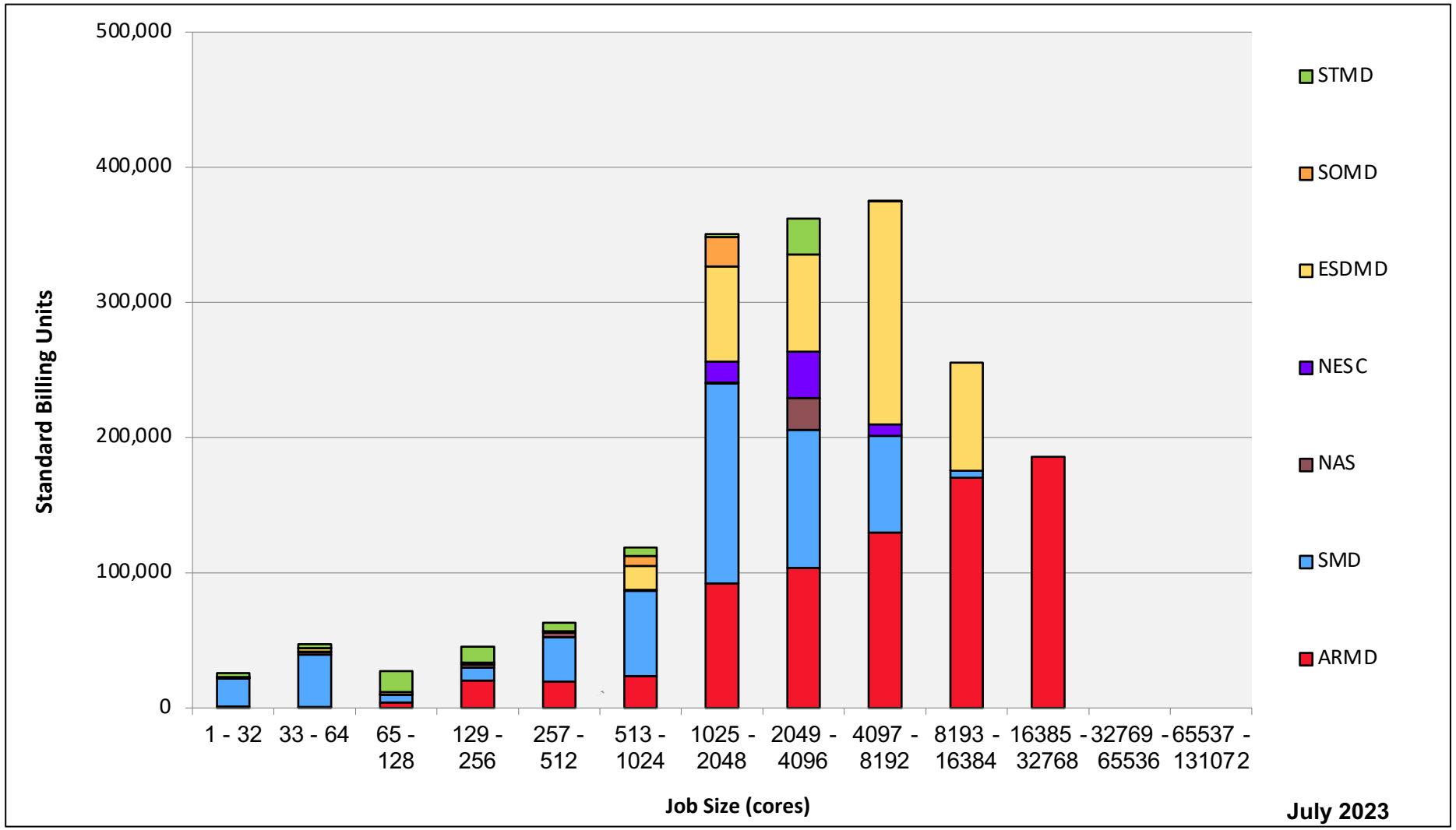
Electra: Devel Queue Utilization



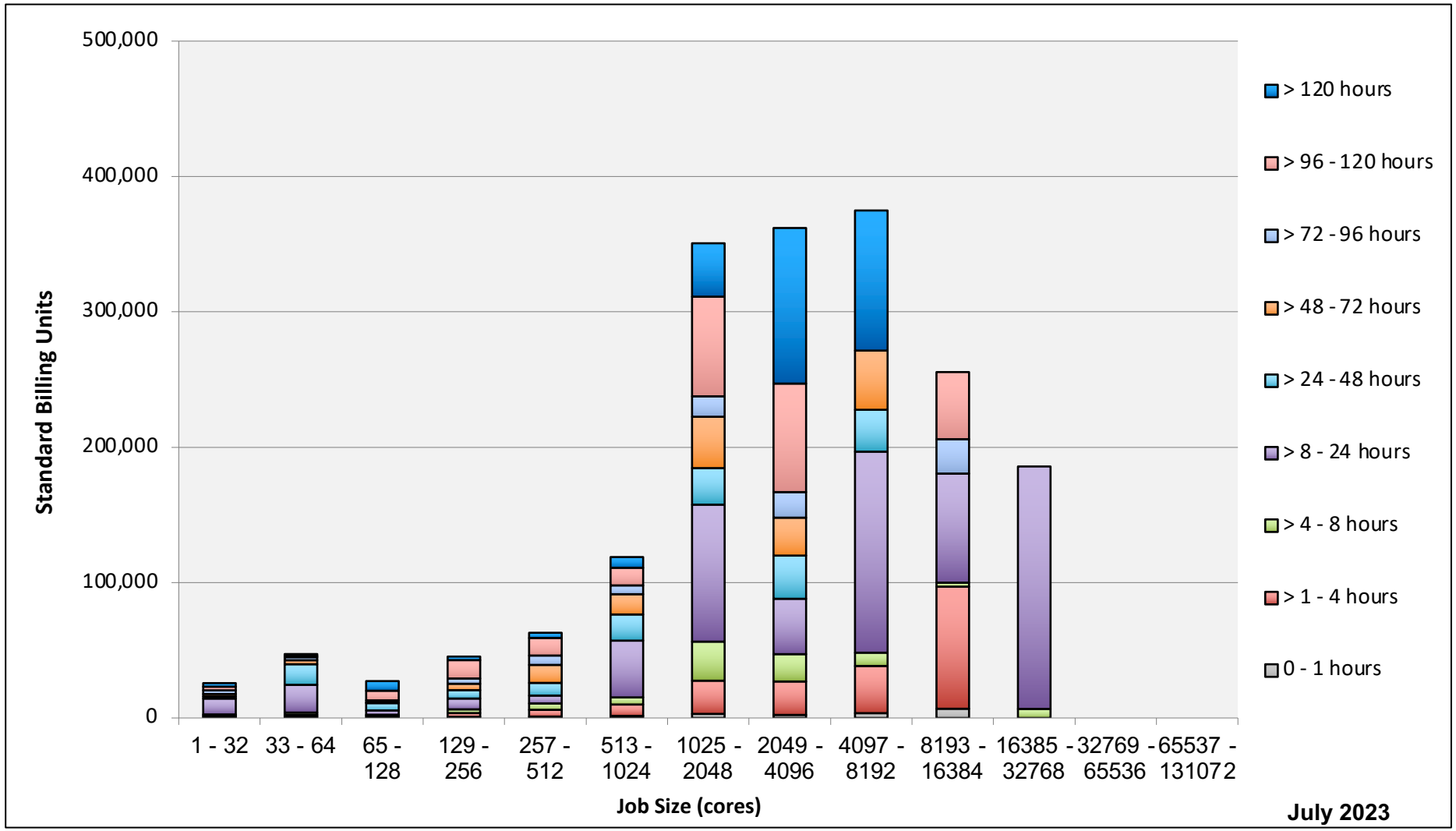
Electra: Monthly Utilization by Job Length



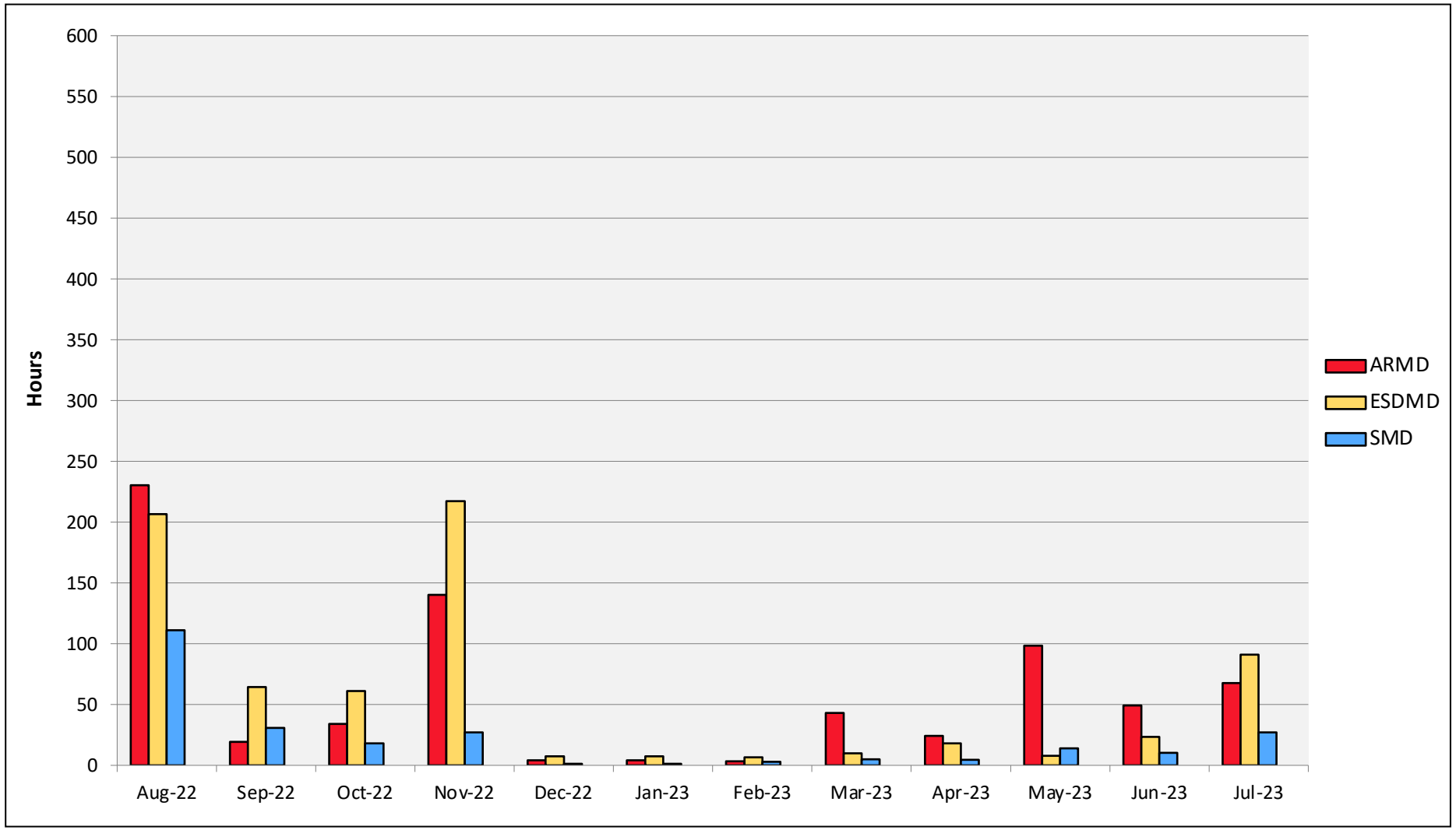
Electra: Monthly Utilization by Job Size



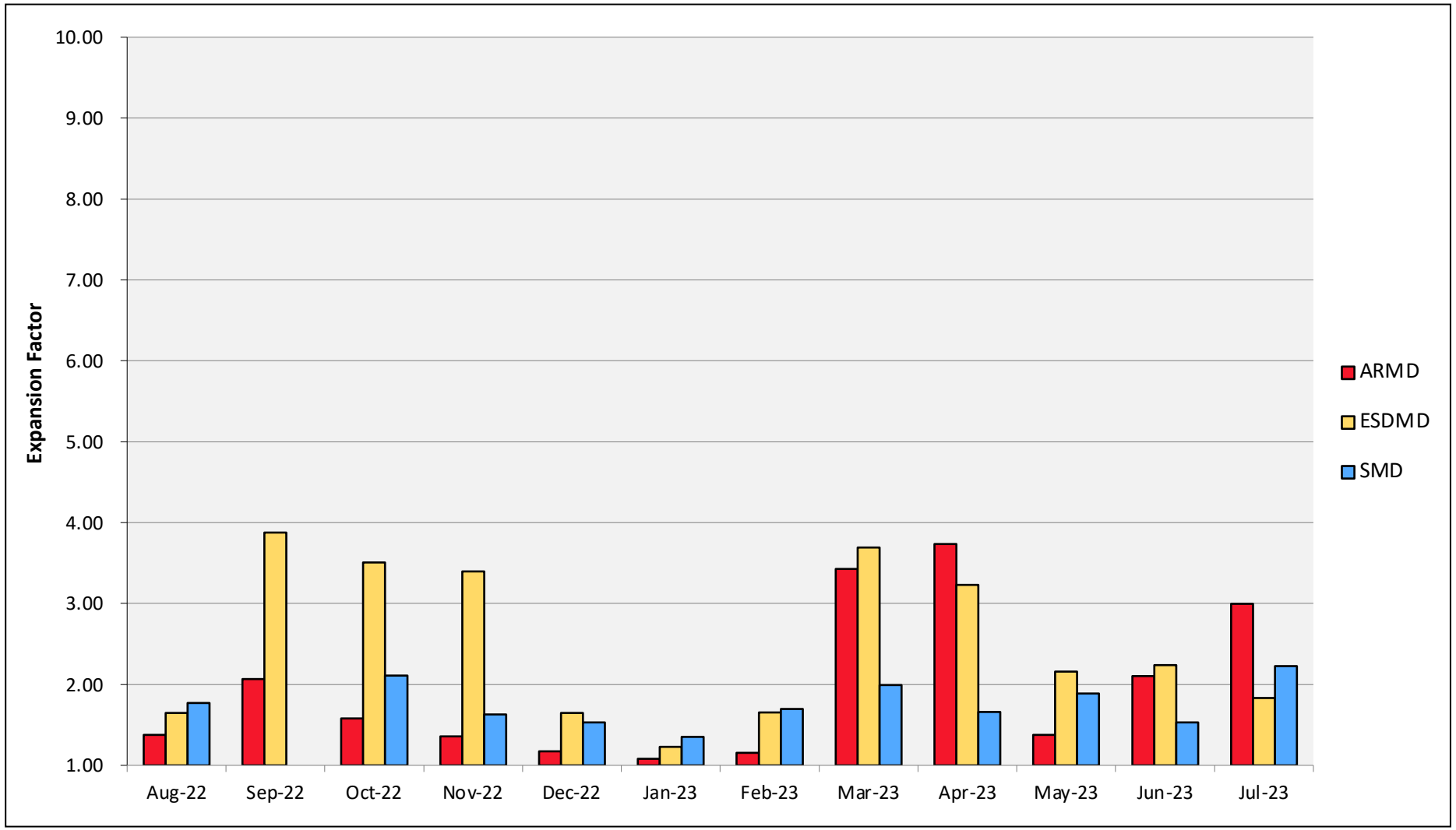
Electra: Monthly Utilization by Size and Length



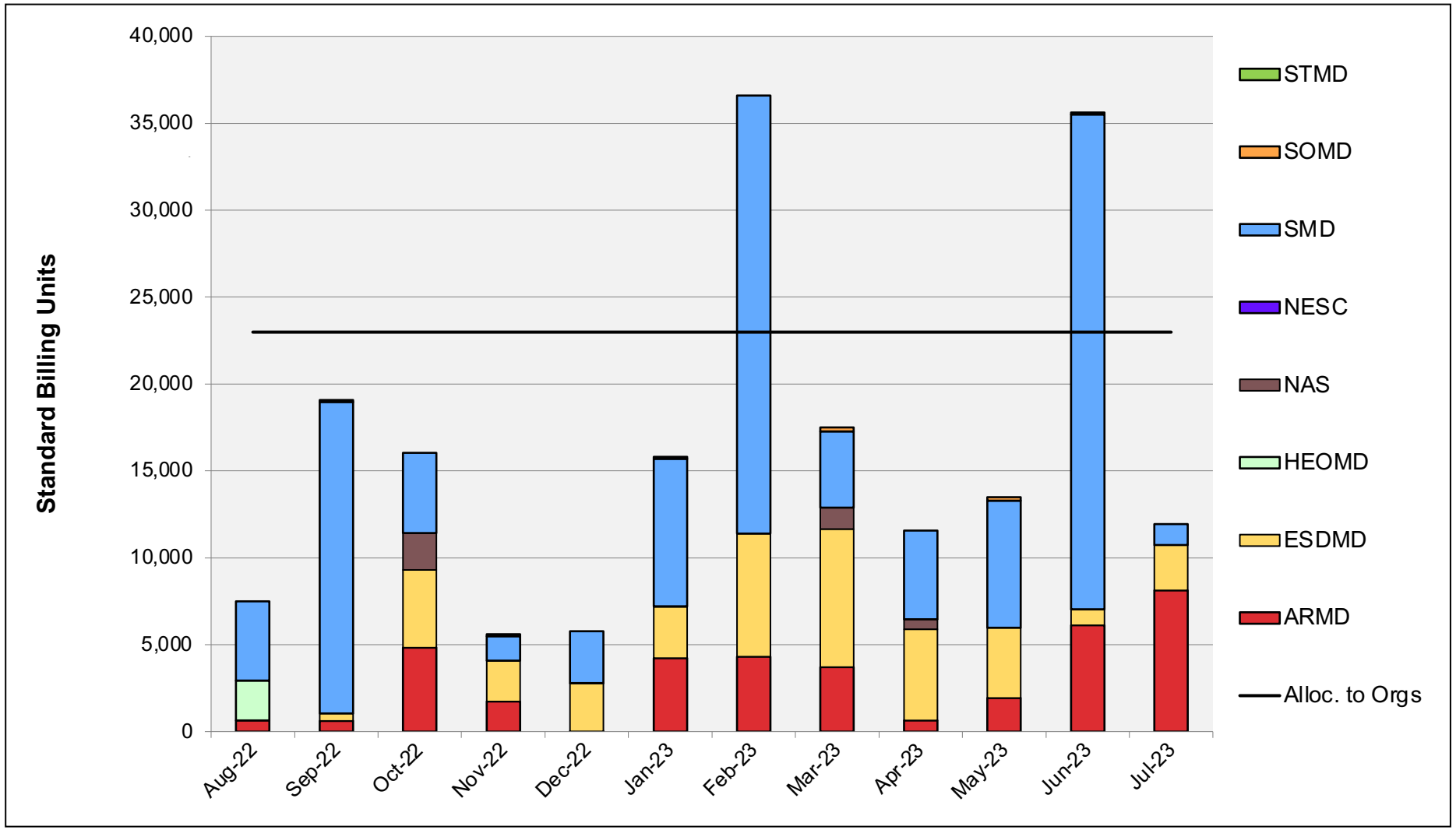
Electra: Average Time to Clear All Jobs



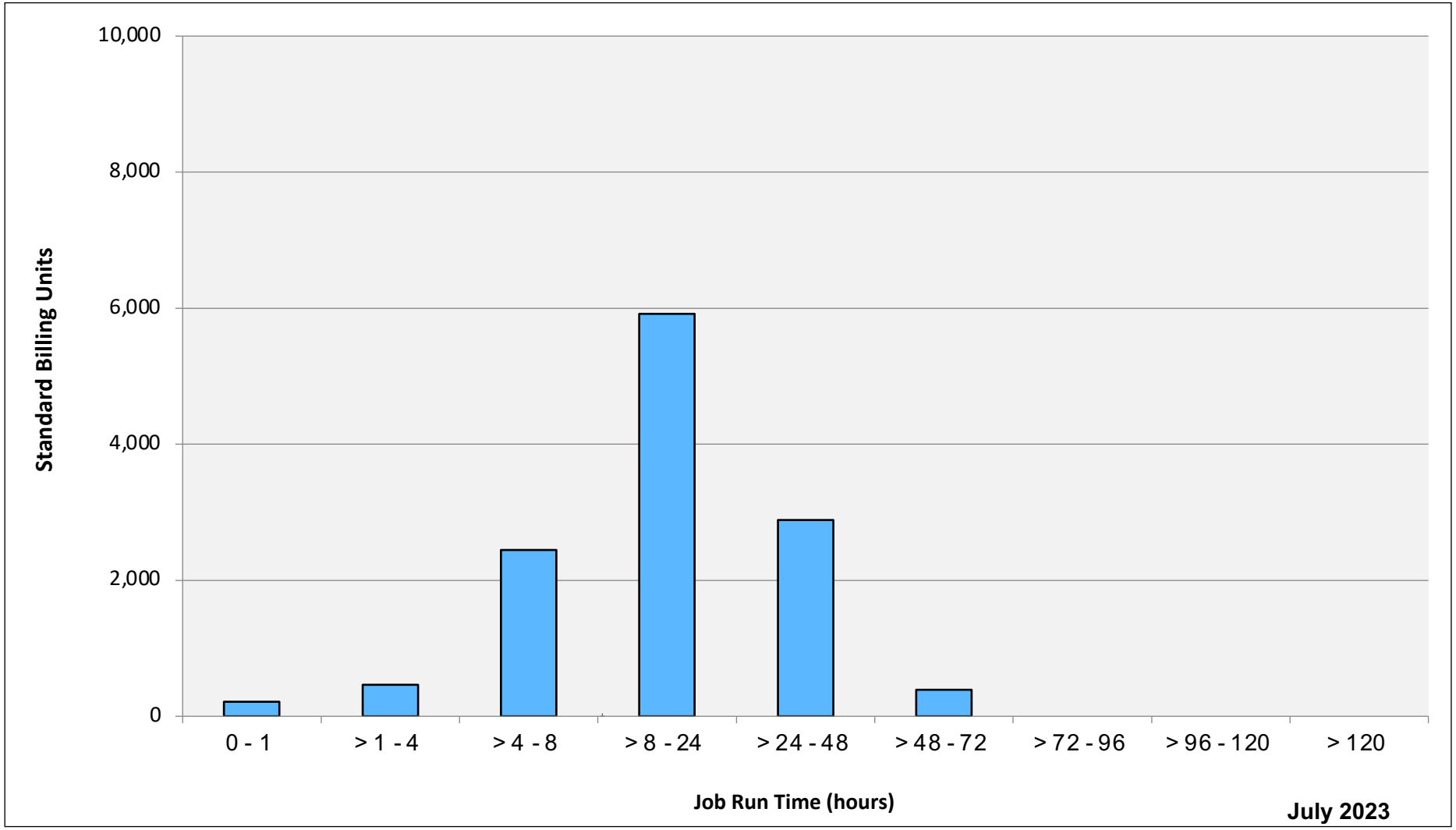
Electra: Average Expansion Factor



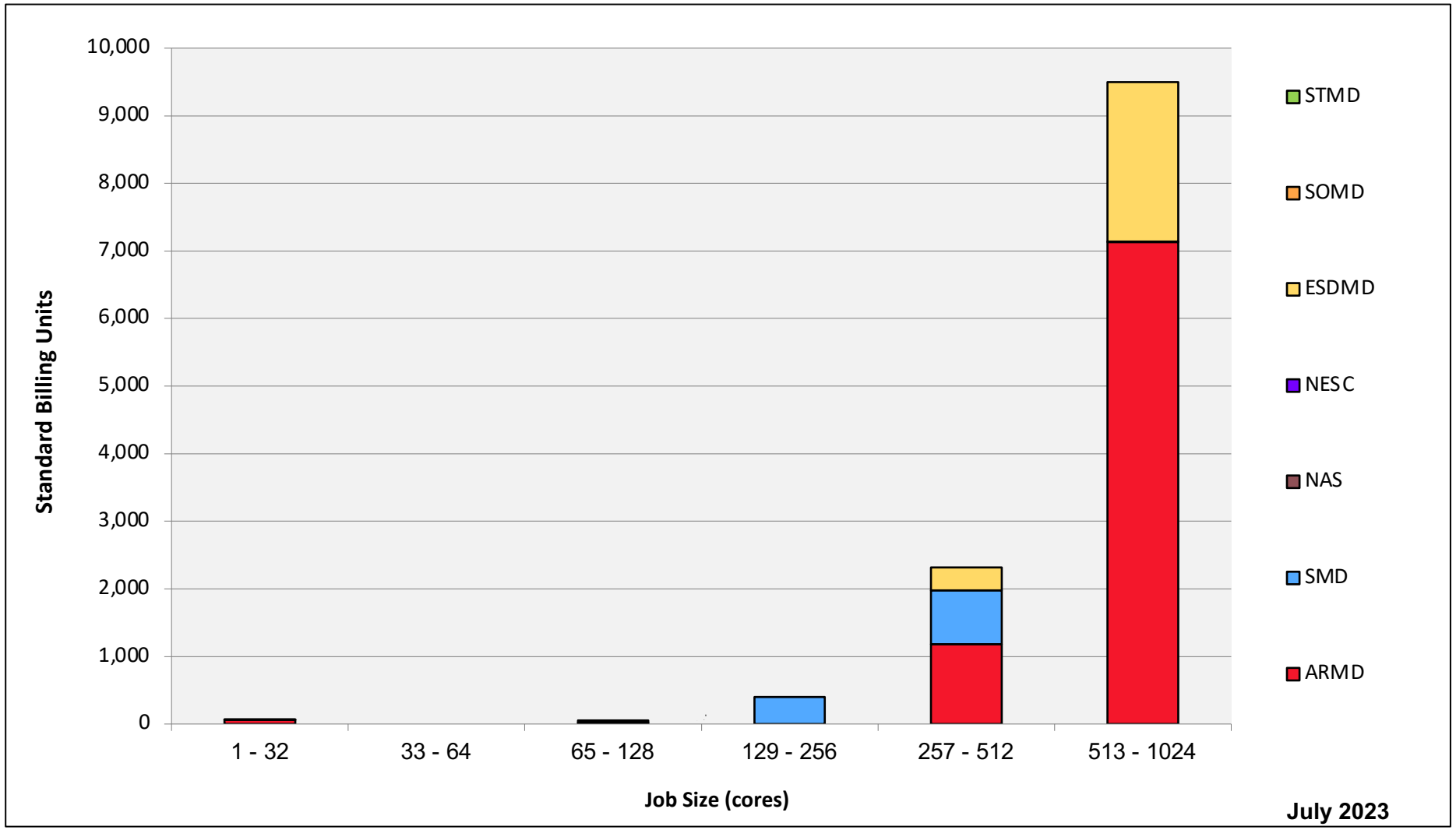
Endeavour: SBUs Reported, Normalized to 30-Day Month



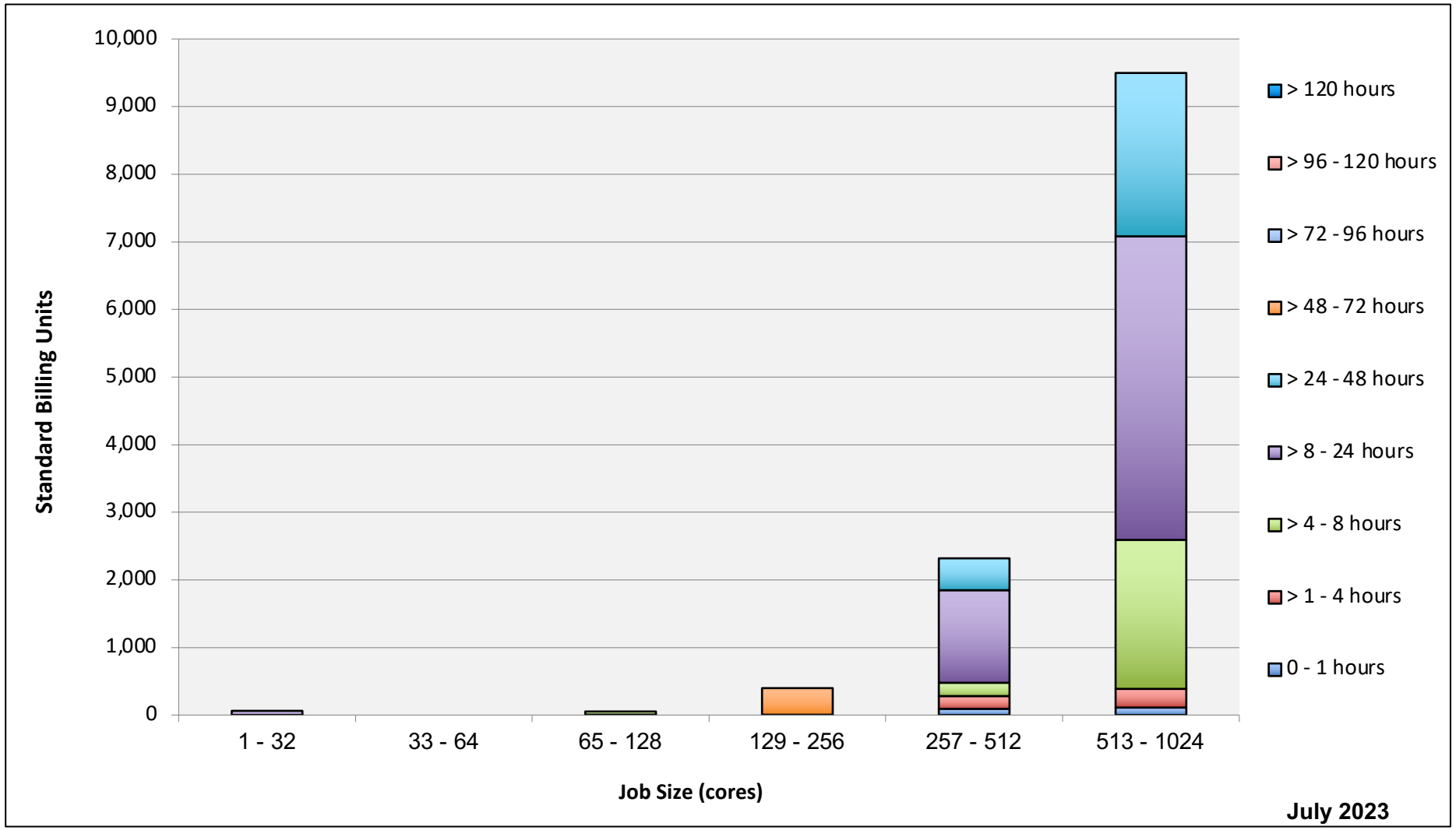
Endeavour: Monthly Utilization by Job Length



Endeavour: Monthly Utilization by Job Size



Endeavour: Monthly Utilization by Size and Length



Endeavour: Average Expansion Factor

