

National Aeronautics and Space Administration

HIGH-END COMPUTING CAPABILITY PORTFOLIO

William Thigpen
NASA Advanced Supercomputing Division

January 10, 2022

Scheduler-Integrated Data Cache Capability Prototype

- In anticipation of NASA's Distributed Active Archives Centers (DAACs) move to the cloud and to meet the agency's future need for hybrid computing and data processing environments, the HECC team prototyped a PBS scheduler-integrated data caching mechanism.
- The effort enables HECC users to use large, diverse datasets from cloud provider infrastructures, such as Amazon Web Services (AWS) Simple Storage Service (S3), more efficiently with the on-prem HPC system.
- The prototyping effort for this milestone included:
  - PBS job prolog directive enhancements: users can specify new directives that will trigger a data pull from select external cloud sources automatically before a job begins.
  - A lazy loading cache strategy: if the data specified in the directive already exists, the job prolog will return immediately or else the system will cache the data for the user.
  - Stale data on local storage (cache) will be cleaned up by the system automatically or as configured reducing overall storage needs.
  - A facility-wide/accessible cache was simulated and tested.
- A facility-wide cache will allow multiple independent users/teams with similar data needs to leverage cloud-based data from the DAACs or other data providers, reducing egress, storage duplication, and overall costs to projects and the agency, while reducing personnel data-wrangling tasks.

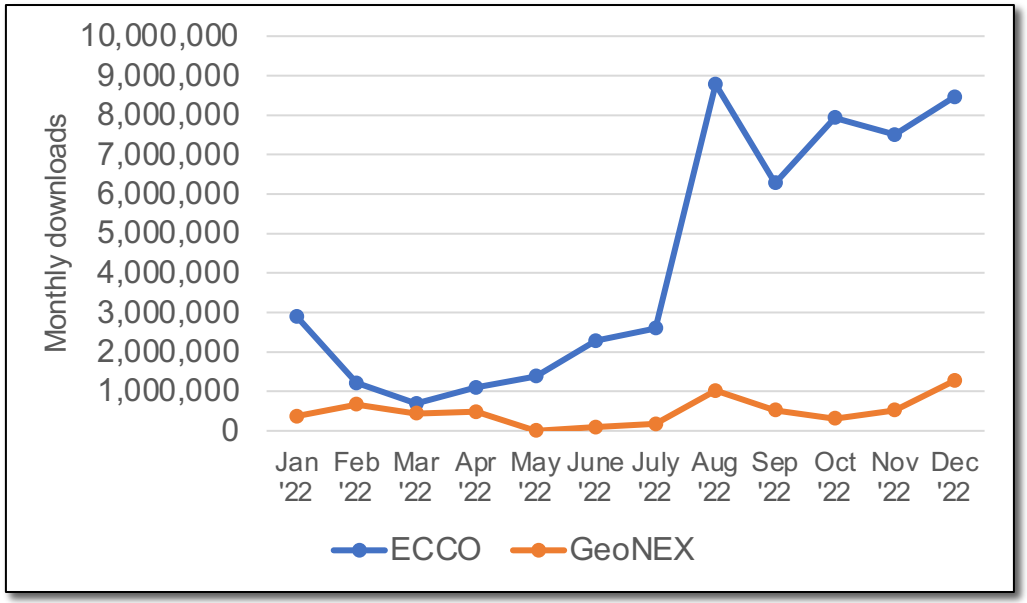
IMPACT: The scheduler-integrated cache capability can 1) reduce agency cloud-based data egress and local storage costs by minimizing duplicate data movements and storage of data standard products; 2) reduce external data access latency for HECC users; 3) improve local resiliency for higher-order workflow systems that drive data intensive processes which may leverage off-prem data sources; and 4) reduce data wrangling for both data staging and local data cleanups with data processing, product generation, and analytics efforts.

User Story: In early December, initial feedback from a NASA Earth Exchange (NEX) user was very positive. A considerable reduction in overall task times, from three weeks to just five days, was achieved using the prototype. The NEX user test utilized 87 terabytes of data and 6,628,350 file objects of Landsat collection 2 data, with the source from an s3://usgs-landsat bucket within the AWS Oregon us-west-2 region, which the USGS EROS Center maintains.

Data Portal Trends and Improvements in 2022

- As the HECC Data Portal community grows, the HECC objective to disseminate scientific data continues to gain traction. During November, the Data Portal site was used by external users to download approximately 250 terabytes of data.
- The portal hit its peak for the most downloaded dataset—ECCO (Estimating the Circulation & Climate of the Ocean)—with more than 8 million downloads in the month of August and 7.5 million file downloads in November 2022.
- GeoNEX, a collaborative effort for generating Earth monitoring products from the new generation of geostationary satellite sensors, came in second in August, at one million downloads.
- During 2022, the Data Portal team improved the reliability of downloads. The team found a pattern of external users/scripts/crawlers not closing connections after a completed download, resulting in system resources waiting for a timeout to close the connection, which decreased the ability for users to download data. Changes to the web server to close these connections resulted in high throughput and a more stable system.

IMPACT: HECC's service of providing public access to scientific datasets through its data portal has seen continuous growth in the number of datasets downloaded.

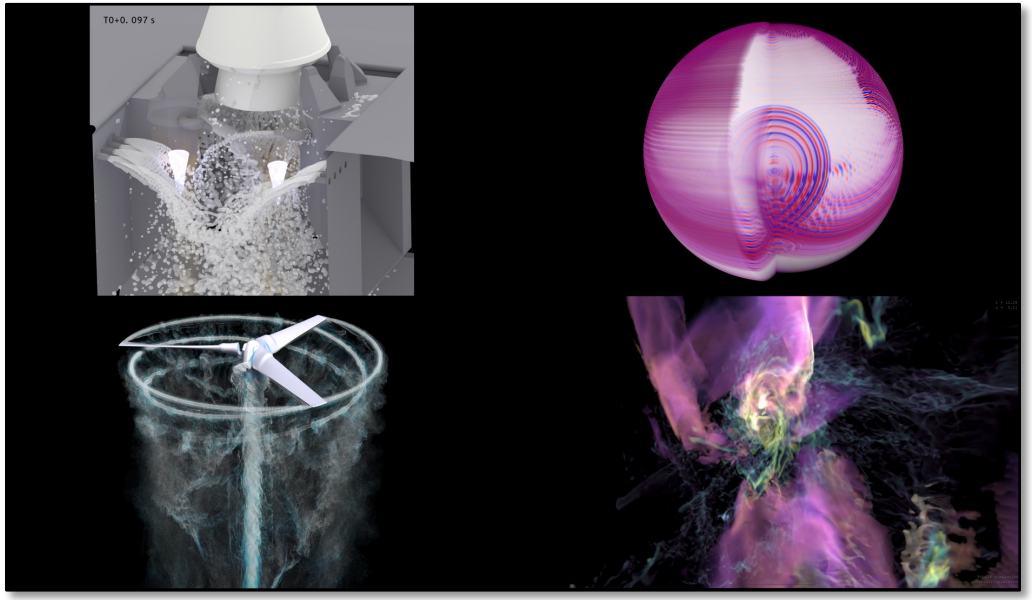


Line graph comparing download metrics for the HECC Data Portal from December 2021 through December 2022. The drop in downloads in September is attributed to a problem with connection closing timeouts. The HECC team's solution is reflected in the increase in October and November 2022.

HECC Visualization Team Support for SC22

- HECC Visualization team members supported numerous researchers for the SC22 conference in November, providing striking animations and images to illustrate and explain their work to attendees and the public.
  - Mission Directorates supported include Human Space Flight, Aeronautics, and Science.
- Support included applying innovative techniques and flexible camera motions and finessing large, time-varying datasets.
  - Volume rendering and ray tracing continue to be a core technology demanded by scientists due to the visual clarity and perception of shape and form conveyed by the lighting and perspective.
  - Massive particle tracing is used to show subtle flow features, such as blade tip vortices, as they propagate through the domain.
- Visualizations often require HECC supercomputing resources to create animations, due to the size or length of a simulation.
  - Jobs often require dozens of high-end compute nodes running overnight to produce one animation.
  - Scientists will often ask for many views, or differing scalar properties, which increases the computational workload.

IMPACT: SC22 visualizations produced by HECC experts allow researchers to communicate their results with a wider audience, inspiring collaboration and innovation.



A sample of the visualizations (shown on the next 4 slides) are provided by HECC Visualization team members: Clockwise from top left: Space Launch System's solid rocket booster plume-water interaction; cross-section of the entire Sun; flow physics of the rotor wake for a V22 Osprey rotor during hover; Figuring Out Gas & Galaxies In Enzo (FOGGIE) galaxies simulation showing gas density of the galaxy disk. *Pat Moran, Nina McCurdy, Tim Sandstrom, and Chris Henze, NASA/Ames.*

HECC hyperwall Display Wall Retired After Extensive Outreach and Scientific Research

- This second hyperwall display was used for 14 years to support analysis of scientific research, inspire scientists and aspiring scientists and to share NASA science and engineering achievements with numerous VIP guests,. The display was retired in December and will be upgraded in 2023 with 4K displays, increasing the resolution by 4x, with more than a billion pixels.
  - VIP guests included NASA Administrators Charles Bolden and Jim Bridenstine, multiple associate administrators and center directors, Special Envoy for Climate John Kerry, the presidents of Brazil and Costa Rica, Governor Schwarzenegger, actor Harrison Ford, and several Congress and Executive branch representatives.
- Custom visual environments were created for the scientific analysis of numerous projects, including:
  - Processed Pressure Sensitive Paint data from the Ames Unitary Plan Wind Tunnel.
  - ECCO 1/48th degree global ocean simulation.
  - Mars climate simulations.
  - Solar simulations.
  - GEOS5-MITgcm coupled atmosphere-ocean global simulation.
  - SETI Institute radio telescope reception event analysis.
  - Sloan Digital Sky Survey search for metal-poor and Lithium-rich stars.
- User comment after using one environment: “One day using this tool equals six months using my workstation.”
- Research conducted when using the hyperwall resulted in at least 11 publications, including five peer-reviewed publications.

IMPACT: The hyperwall enabled the analysis of NASA science and engineering results, and the dissemination of those results within the agency and to the public.

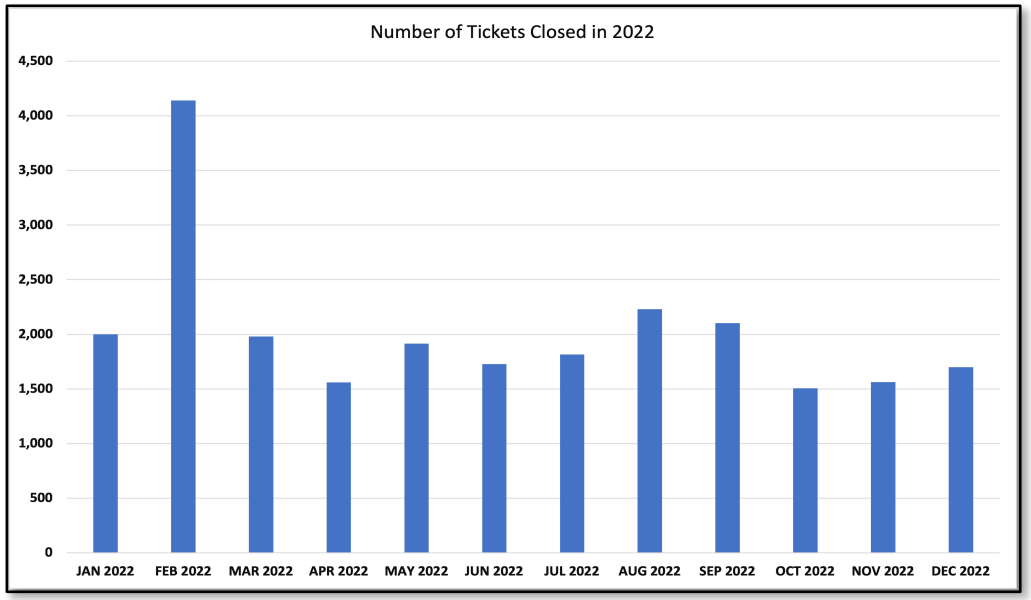


Working sessions while using three different visualization environments on the HECC hyperwall. Top left and right: ECCO ocean simulation (*David Ellsworth, NASA/Ames*). Bottom left: Pressure Sensitive Paint (*Nettie Roozeboom*). Bottom right: Solar simulation (*Patrick Moran, NASA/Ames*).

Control Room Staff Provides Essential Services to Users

- In 2022, HECC Control Room analysts (CRAs) provided support to more than 1,800 users from all of NASA's mission directorates. CRAs processed, tracked, and resolved over 25,500 tickets for the 12 months from January 1 through December 31.
- Tickets covered a wide range of support activities—from automated notifications of system issues to resolving a variety of issues for users calling for help:
  - Answered inquiries about accounts, failed jobs, and status of systems.
  - Extended the runtimes of already-queued or running jobs.
  - Created complex reservations for mission-critical projects.
  - Modified allocations and account expiration dates.
  - Explained file transfer tools and processes.
  - Debugged job failures and identified execution bottlenecks.
- Another significant accomplishment during 2022 was the creation and implementation of structured Standard Operating Procedures (SOP) for Control Room tasks. The SOPs include Owner/Author, Subject Matter Expert (SME) review, peer review, revision numbers and dates, and bi-annual review. The SOPs allow for faster CRA integration and expertise within the HECC organization, providing better customer support and experience.
  - 30 SOPs are published within the Remedy Knowledge Base.
  - 23 SOPs drafts are in progress/review.

IMPACT: The 24x7 support services provided by HECC Control Room analysts resolve system problems and users' technical issues and enable users to focus on their important mission projects.

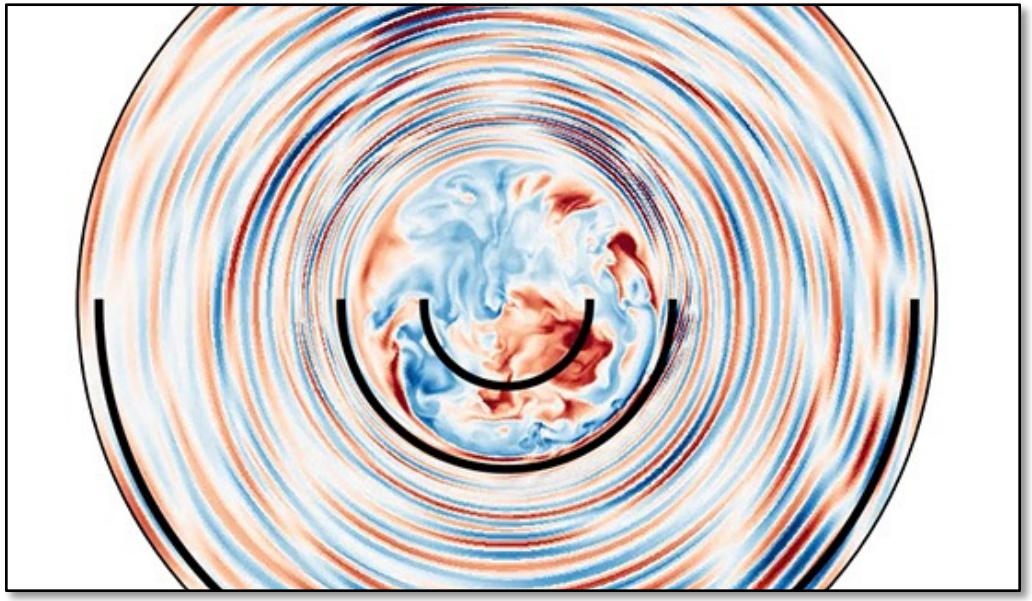


HECC Control Room staff resolved, on average, more than 2,125 Remedy tickets per month in 2022—just over 25,500 tickets total.

Simulations Lead to New Findings in Solar Magnetic Cycles and Waves*

- Running simulations on HECC resources, researchers at Northwestern University made several discoveries in their quest to understand how the Sun's magnetic fields are built and how convective flows generate waves that propagate to the surface.
  - Prendergast magnetic field configurations—previously believed to be stable—are unstable, so magnetic equilibrium solutions may be more difficult to obtain.
  - Some solar and stellar dynamos are linked to the magneto-rotational instability if there is sufficient radial differential rotation, showing an alternative path for stellar dynamo theory.
- Recent 3D simulations captured penetrative rotating convection, the wave excitation region, and wave propagation to estimate their surface amplitudes, which allowed researchers to compare their results to stellar observations.
- HECC resources enable work with Dedalus, a flexible and spectral framework for solving several classes of problems
- HECC applications experts optimized parts of the Dedalus code to run these simulations on NAS facility resources and to build software stacks that support many users.

IMPACT: HECC resources and code experts enable high-resolution 3D simulations that support NASA's goals to understand how the universe works, along with helping protect our technology and astronauts in space.



The nature of waves driven by core convection, examined with 3D fully compressible spherical simulations of a model star containing a convective core and a stable radiative envelope. *Evan Anders, CIERA Northwestern University*

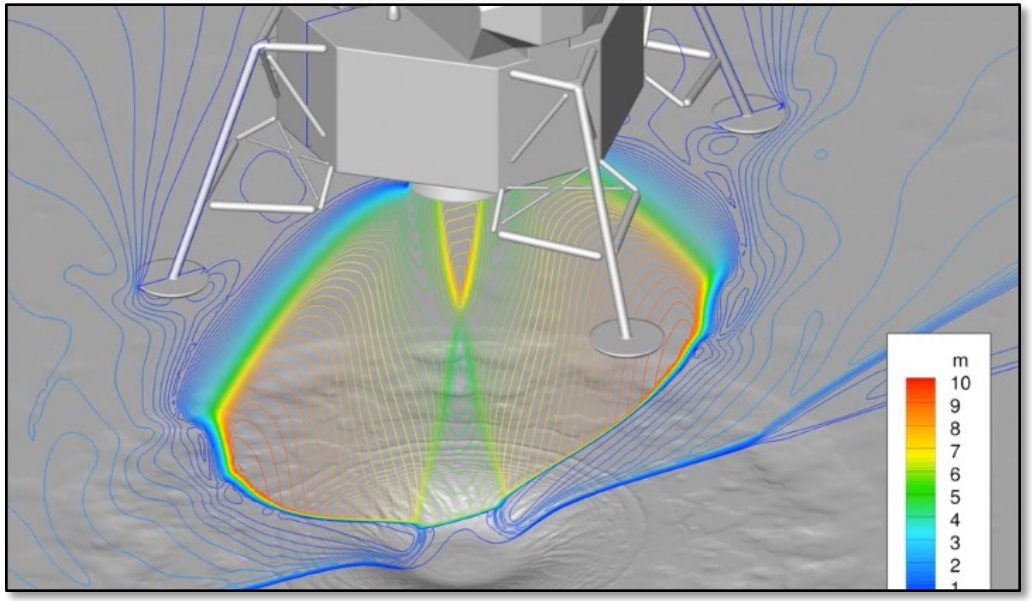
** HECC provided supercomputing resources and services in support of this work.*

Plume-Surface Simulations for Moon and Mars Landings*

- Plume-surface interaction (PSI) between a lander's engine plumes and regolith (the fine soil found on solid planetary bodies) creates many hazards during landing, including obscuration, contamination, high-energy ejecta streams, and landing area cratering.
- The Fluid Dynamics Branch at Marshall Space Flight Center (MSFC) developed simulation tools to provide PSI environment predictions to teams across the agency, including those working on the Human Lander System, Commercial Lunar Payload Services, and future crewed Mars landers.
- Their gas-particle multi-phase interaction modeling of surface erosion was run on HECC systems to predict erosion, crater formation, and particle streams, with particular attention to proper modeling of the roughness and interlocking of real particle shapes and sizes. Models were validated against low atmosphere and vacuum experiments, and Apollo lunar landing observations.
- The team's simulations demonstrated that a rocket plume expanding into a very low pressure atmosphere affects the surface impingement forces with significant influence in the liberation of surface material; and show the importance of the particle roughness and size distribution–features that can resist the penetration of gas flow and reduce erosion.
- These simulations required over one hundred million cells and 4,000–8,000 cores on the HECC supercomputers, running 2–4 weeks each.

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

IMPACT: This work is providing insight into the plume structure dynamics and the significance of flow effects in surface erosion, giving future lander missions vital information to assure safety to vehicles, science payloads, and crew during solid-surface planetary landings.



Apollo Lunar Module cratering simulations were performed using the Gas-Granular Flow Solver (GGFS) with the nozzle exit five meters above ground. The image shows a plume-induced crater evolution for a tri-disperse sphere particle mixture with 10/30/100-micron particle sizes. *Peter Liever, NASA/Marshall*

Papers

- "**Effects of Thermophoresis on High-Pressure Binary-Species Boundary Layers with Uniform and Non-Uniform Compositions**," T. Toki, J. Bellan, Journal of Fluid Mechanics, vol. 952, December 1, 2022. * *https://www.cambridge.org/core/journals/journal-of-fluid-mechanics/article/abs/effects-of-thermophoresis-on-highpressure-binaryspecies-boundary-layers-with-uniform-and-nonuniform-compositions/175DC83A770F3CA1D2FD23F921E6EB0C*
- "**Molecular Dynamics Simulations of Austenite-Martensite Interface Migration in NiTi Alloy**," G. Plummer, et al., Physical Review Materials, vol. 6, published online December 5, 2022. * *https://journals.aps.org/prmaterials/abstract/10.1103/PhysRevMaterials.6.123601*
- "**Do Submesoscales Affect the Large-Scale Structure of the Upper Ocean?**" A. Sinha, J. Callies, D. Menemenlis, Journal of Physical Oceanography, published online December 5, 2022. * *https://journals.ametsoc.org/view/journals/phoc/aop/JPO-D-22-0129.1/JPO-D-22-0129.1.xml*
- "**TESS Hunt for Young and Maturing Exoplanets (THYME) IX: A 27 Myr Extended Population of Lower-Centaurus Crux with a Transiting Two-Planet System**," M. Wood, et al., arXiv:2212.03266 [astro-ph.SR], December 6, 2022. * *https://arxiv.org/abs/2212.03266*
- "**A Global Simulation of the Dynamo, Zonal Jets, and Vortices on Saturn**," R. K. Yadav, et al., The Astrophysical Journal, vol. 940, no. 2, December 6, 2022. * *https://iopscience.iop.org/article/10.3847/1538-4357/ac9d94/meta*

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

Papers (cont.)

- "**Search for Planets around Stars with Wide Brown Dwarfs**," J. Šubjak, et al., arXiv:2212.03757 [astro-ph.EP], December 7, 2022. *
  https://arxiv.org/abs/2212.03757
- "**An Improved Magentohydrodynamic Simulation of the 2006 December 13, Coronal Mass Ejection of NOAA Active Region 10930**," Y. Fan, The Astrophysical Journal, vol. 941, no. 1, December 13, 2022. *
  https://iopscience.iop.org/article/10.3847/1538-4357/aca0ec/meta
- "**Impact Induced H_2-rich Climates on Early Mars Explored with a Global Climate Model**," K. Steakley, et al, Icarus, vol. 394, published online December 15, 2022. *
  https://www.sciencedirect.com/science/article/pii/S0019103522004936
- "**Energy Deposition by Mesoscale High-Latitude Electric Fields into the Thermosphere During the 26 October 2019 Geomagnetic Storm**," X. Meng, et al., Journal of Geophysical Research: Space Physics, vol. 127, issue 12, December 15, 2022. *
  https://agupubs.onlinelibrary.wiley.com/doi/full/10.1029/2022JA030716
- "**Numerical Study of Magnetic Island Coalescence Using Magnetohydrodynamics with Adaptively Embedded Particle-in-Cell Model**," D. Li, et al., arXiv:2212.07980 [physics.plasm-ph], December 15, 2022. *
  https://arxiv.org/abs/2212.07980

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

Papers (cont.)

- "**Spinning up a Daze: TESS Uncovers a Hot Jupiter Orbiting the Rapid-Rotator TOI-778**," J. Clark, et al., arXiv:2212.08242 [astro-ph.EP], December 16, 2022. *
  https://arxiv.org/abs/2212.08242
- "**Occurrence Rate of Hot Jupiters Around Early-type M Dwarfs Based on Transiting Exoplanet Survey Satellite Data**," T. Gan, et al., The Astrophysical Journal, vol. 165, no. 1, December 16, 2022. *
  https://iopscience.iop.org/article/10.3847/1538-3881/ac9b12/meta
- "**Characterizing Observed Extra Mixing Trends in Red Giants using the Reduced Density Ratio from Thermohaline Models**," A. Fraser, et al., The Astrophysical Journal, vol. 941, no. 2, December 20, 2022. *
  https://iopscience.iop.org/article/10.3847/1538-4357/aca024/meta
- "**Human Health during Space Travel: State-of-the-Art Review**," C. Krittanawong, et al., Cells: Research Advances Related to Cardiovascular System (Special Issue), December 22, 2022. *
  https://www.mdpi.com/2073-4409/12/1/40

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

Presentations

- **American Geophysical Union (AGU) Fall Meeting 2022**, Chicago, IL, December 12-16, 2022.
  - "**Radiation Data Portal: Enhancing Data Discoverability and Analysis for Understanding Space Radiation in Earth Environment**," V. Sadykov, Z. Watkins, D. Kempton, X. He, W. K. Tobiska, C. Mertens, S. Ranjan, I. Kitiashvili, R. Spaulding, G. Deardorff.
    https://agu.confex.com/agu/fm22/meetingapp.cgi/Paper/1157001
  - "**Contribution to Solar Brightness of Small-Size Magnetic Elements**," V. Sadykov, S. Criscuoli, S. Bahauddin, D. Erfani, M. Faurobert, I. Kitiashvili, M. Rast, C. Peck, M. Rempel, M. Snow, A. Tritschler, C. Laughrey.
    https://agu.confex.com/agu/fm22/meetingapp.cgi/Paper/1071684
  - "**Unexpected Phase-Shifts of Acoustic Waves Observed in Read Data as well as in Simulations and Their Impact on Estimations of the Deep Meridional Flow**," M. Waidele, J. Zhao, I. Kitiashvili.
    https://agu.confex.com/agu/fm22/meetingapp.cgi/Paper/1097387
  - "**Fine Structure of Near-Surface Rotational Shear Layer in 3D Radiative Hydrodynamics Simulations of the Solar Convection Zone**," I. Kitiashvili, A. Kosovichev, A. Wray, V. Sadykov, G. Guerrero.
    https://agu.confex.com/agu/fm22/meetingapp.cgi/Paper/1093866
  - "**Updates in Developing a Prototype Science Pipeline and Full-Volume, Global Hyperspectral Synthetic Data Sets for NASA's Earth System Observatory's Upcoming Surface, Biology, and Geology Mission**," J. Jenkins, P. Tenenbaum, Y. Shinozuka, B. Wohler, A. Michaelis, J. Dungan, I. Brosnan, V. Genovese, W. Wang, M. Gierach, P. Townsend, B. Poulter, A. Chlus.
    https://agu.confex.com/agu/fm22/meetingapp.cgi/Paper/1075223
- "**How Supercomputing Supports NASA's Mission**," P. Mehrotra, U.S. Competitiveness in the Global HPC Market: Recent Changes, Concerns, and the Potential Impacts from the CHIPS and Science Act**,** Washington D.C., December 13, 2022.
  https://hyperionresearch.com/wp-content/uploads/2022/12/NASA_P.-Mehrotra_Hyperion-Research-DC-event-12.13.22.pdf

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

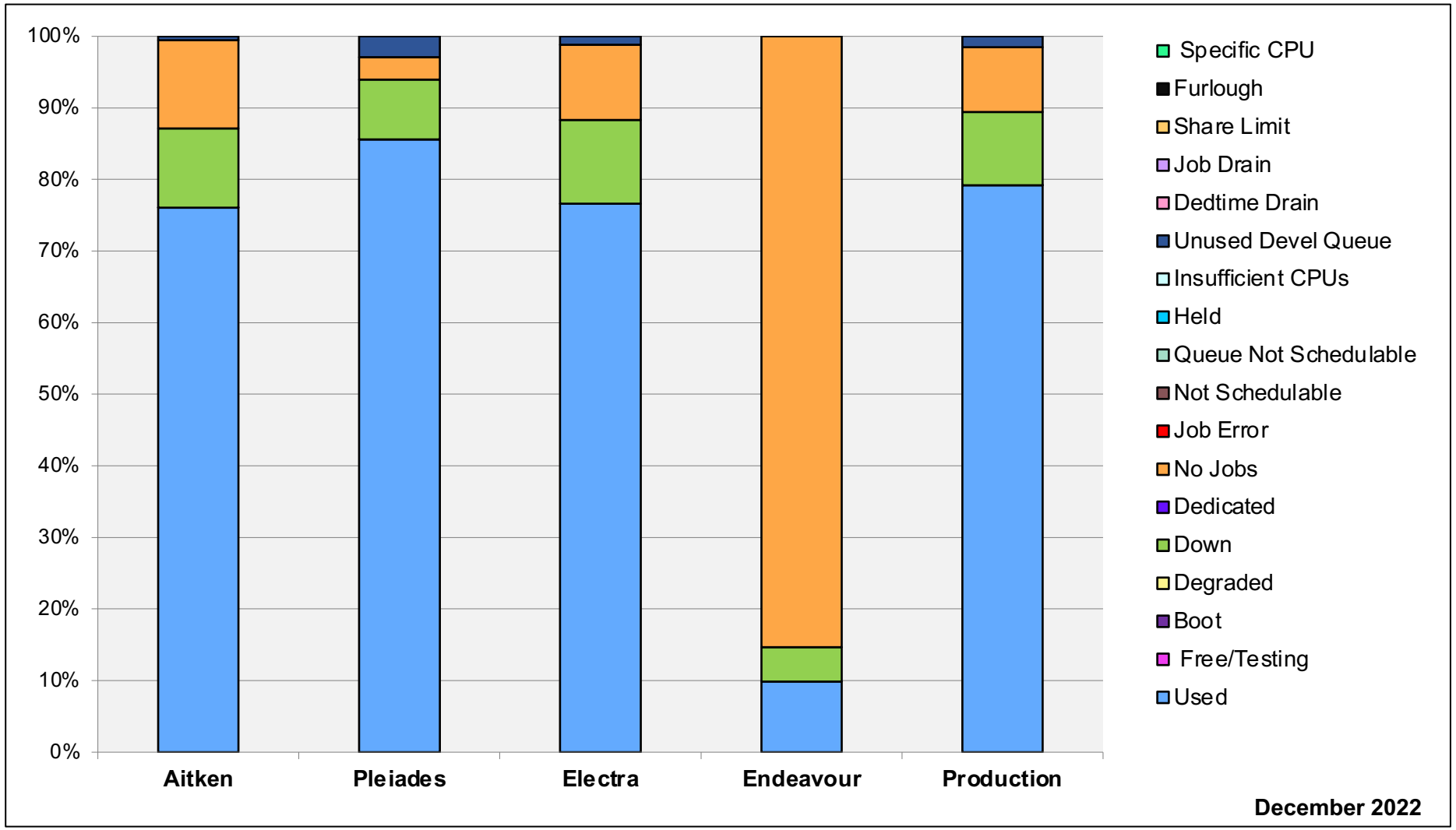
News and Events

- **The Gift that Keeps on Giving: NAS Division Research in 2022***, NAS Feature,* December 20, 2022—Launch pad safety. Mars landings. Cleaner, quieter aircraft. Fourteen selected projects led by NAS Division experts over the past year will benefit agency missions and projects for years to come! All were presented during SC22, the International Conference for High-Performance Computing, Networking, Storage, and Analysis, where NASA returned in person this year to showcase the science and engineering made possible by the agency's supercomputers. *https://www.nas.nasa.gov/pubs/stories/2022/feature_SC22_wrap_Dec_22.html*
- **The World's Largest Turbulence Simulation Unmasks the Flow of Energy in Astrophysical Plasmas**, *Princeton Plasma Physics Laboratory*, December 23, 2022—Researchers uncovered a previously hidden heating process that helps explain how the atmosphere that surrounds the Sun can be vastly hotter than the solar surface that emits it. The discovery could improve how we tackle a range of astrophysical puzzles, such as star formation, the origin of large magnetic fields in the universe, and our ability to predict eruptive space weather events. *https://www.pppl.gov/news/2022/worlds-largest-turbulence-simulation-unmasks-flow-energy-astrophysical-plasmas*

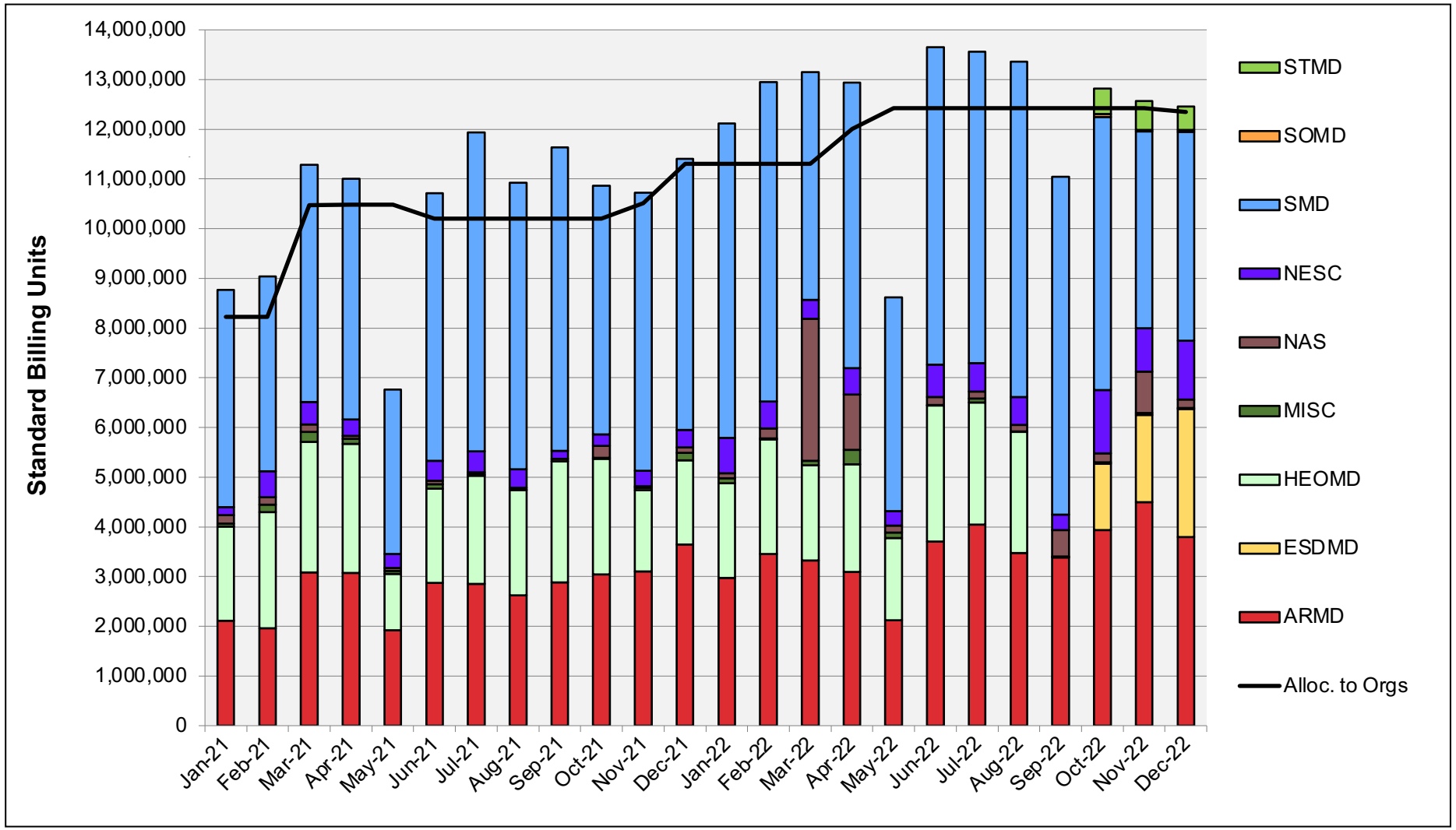
News and Events: Social Media

- **Coverage of NAS Stories**
  - 2022 Wrap-Up Story:
    - NAS: Twitter 17 retweets, 2 quote tweets, 99 likes.

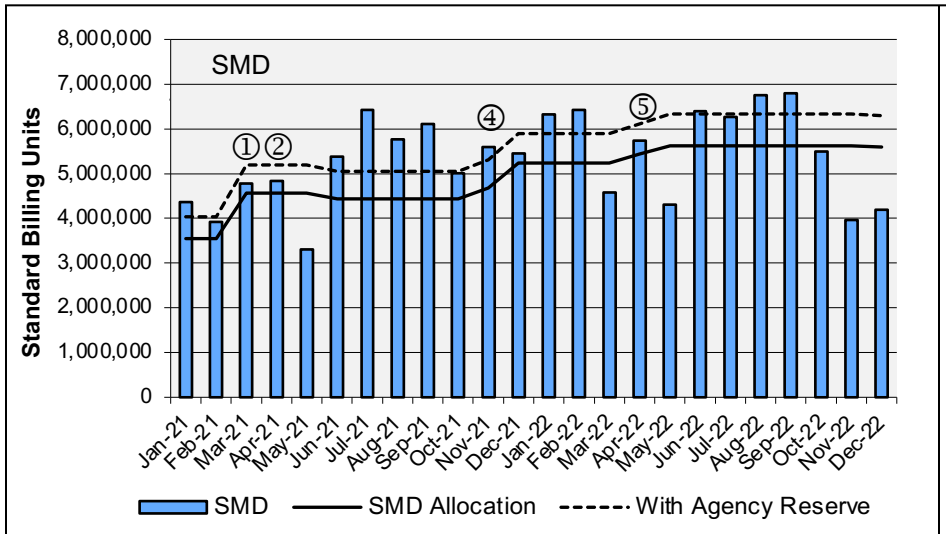
HECC Utilization

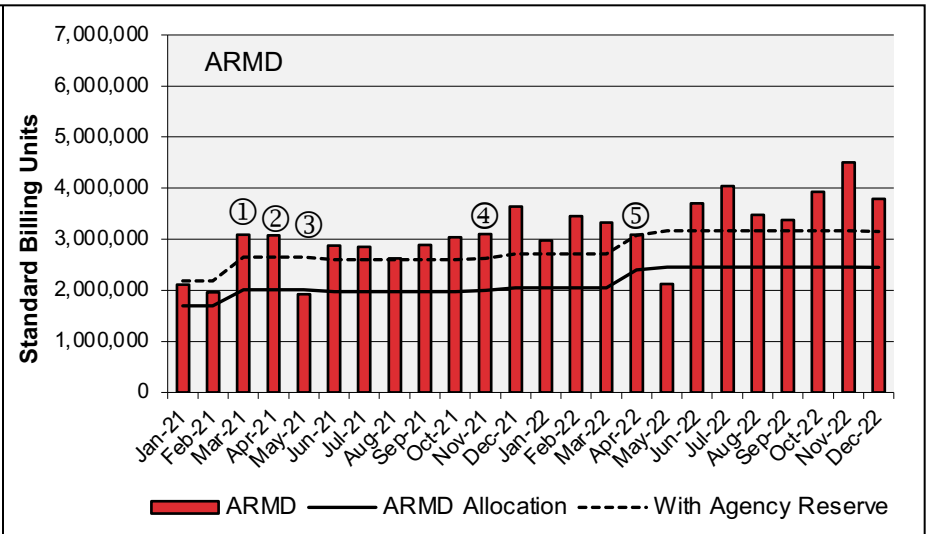


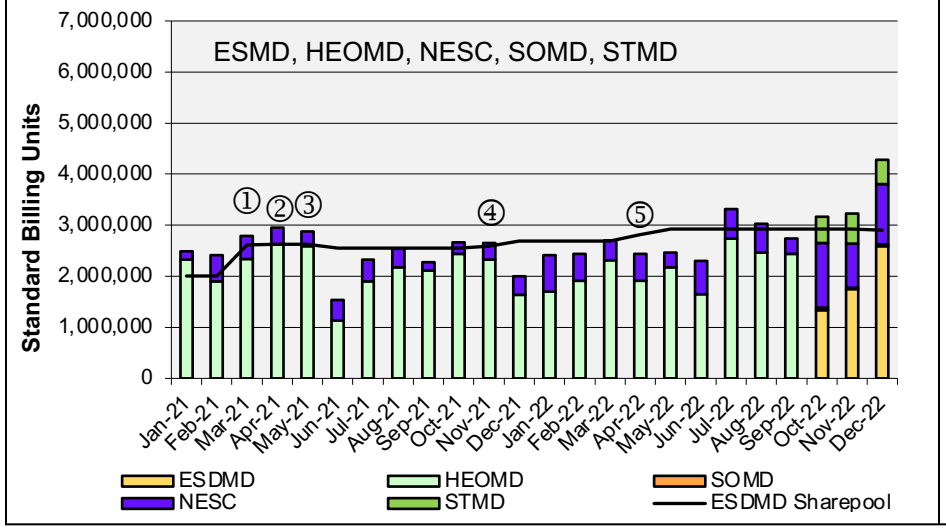
HECC Utilization Normalized to 30-Day Month



HECC Utilization Normalized to 30-Day Month







① 8 Rome Apollo racks introduced into Aitken

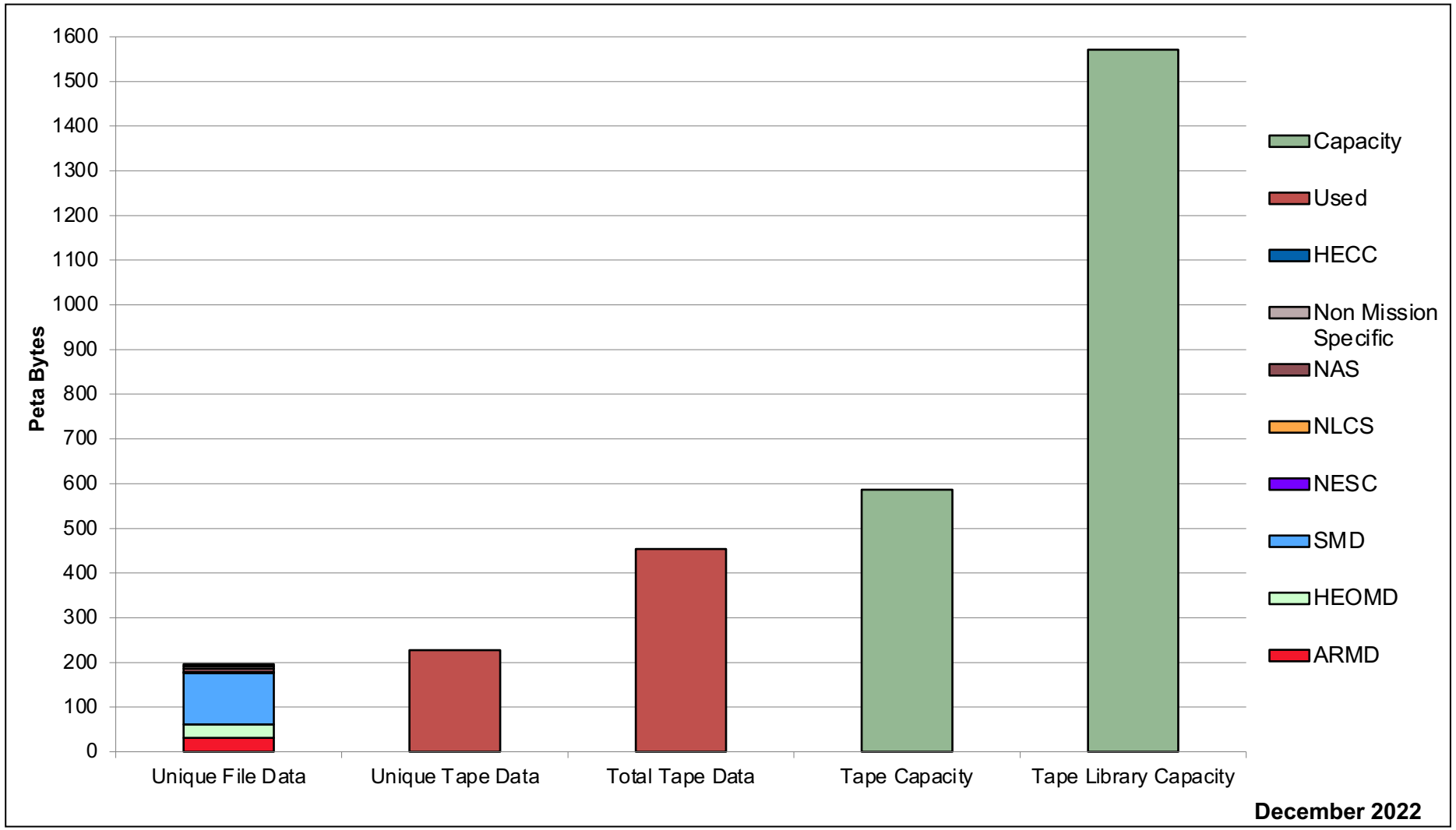
② Endeavour replaced with new hardware

③ Merope retired

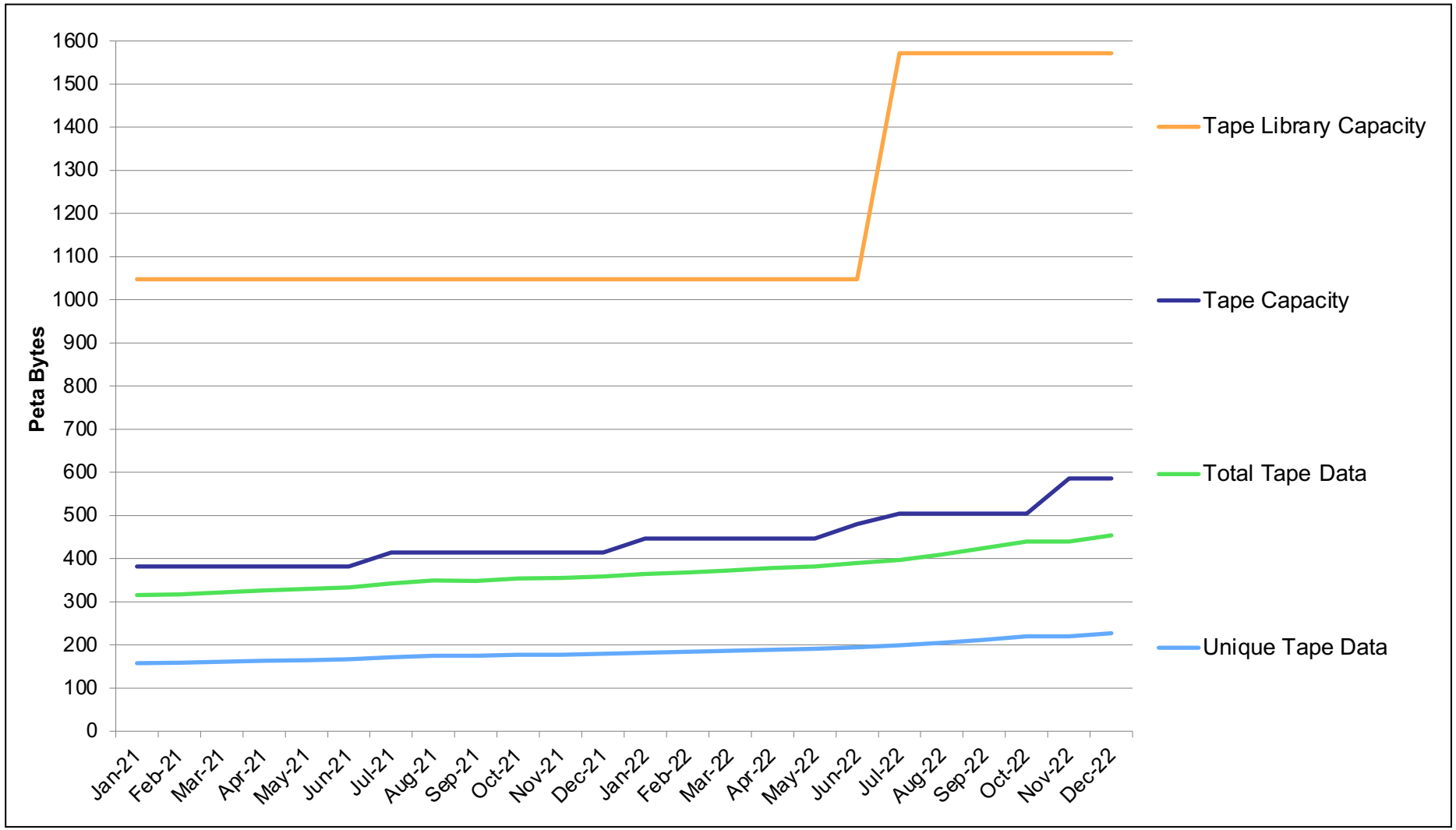
④ 4 Rome Apollo Racks added to Aitken

⑤ 4 Rome Apollo Racks added to Aitken

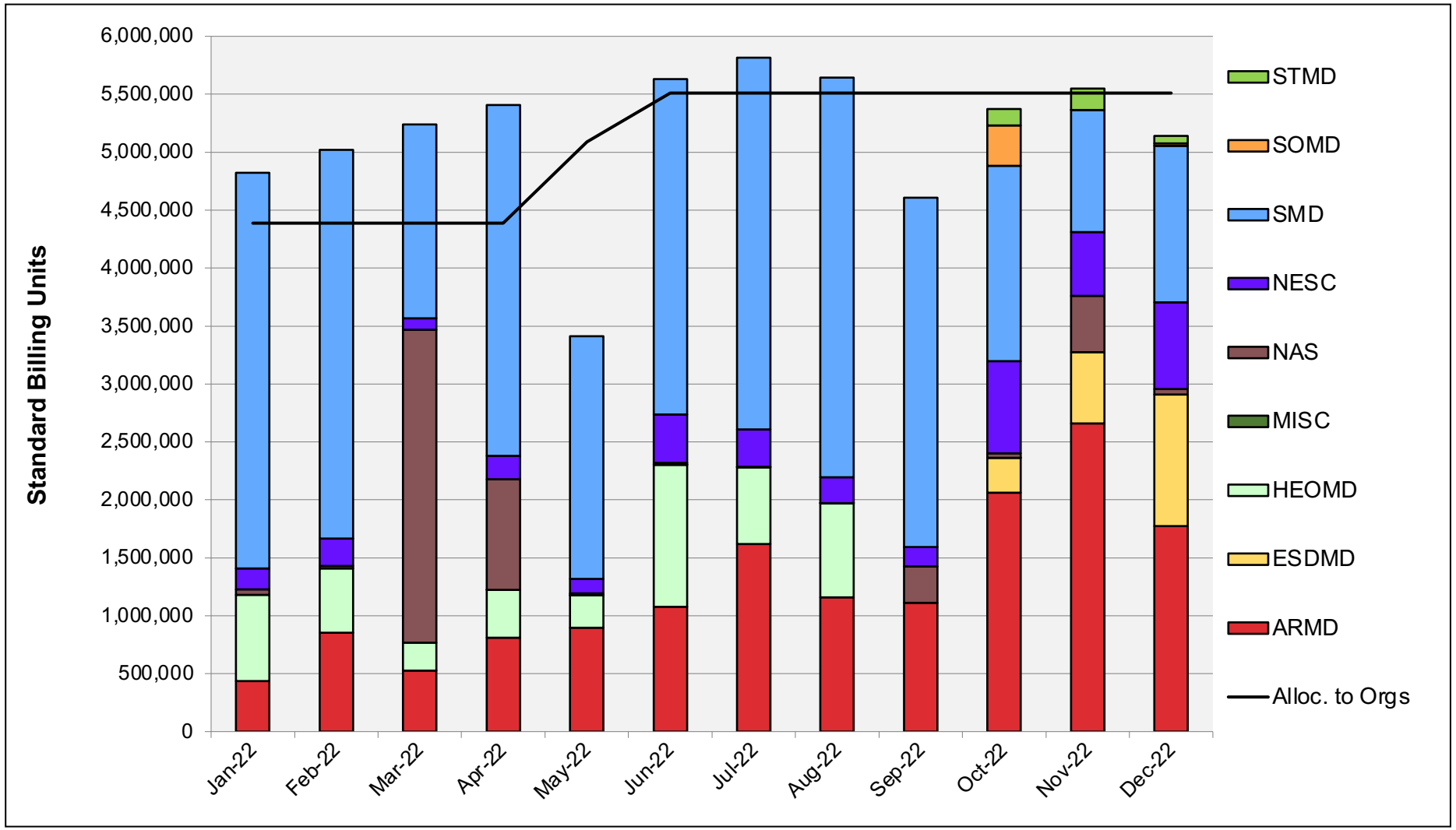
Tape Archive Status



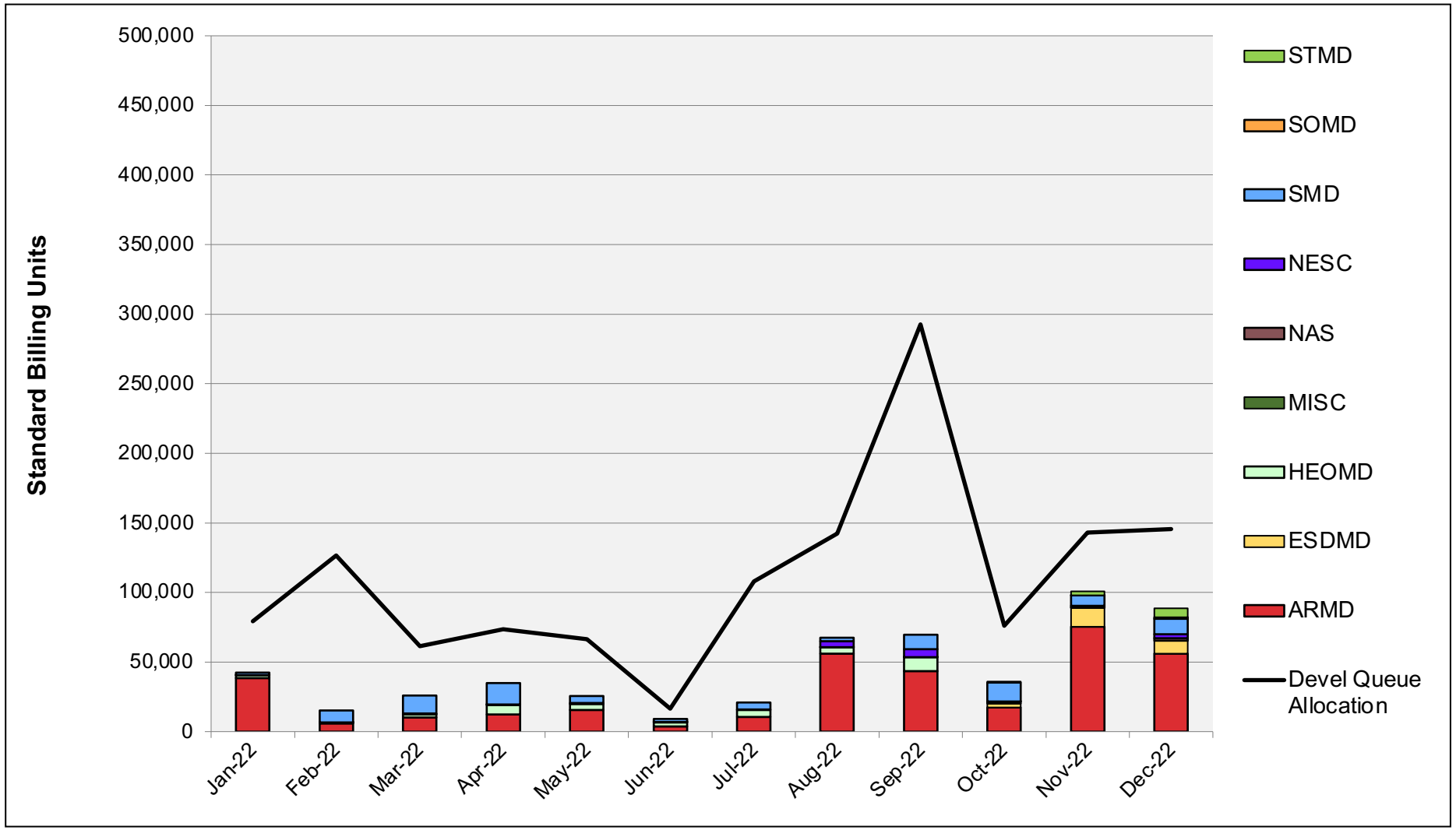
Tape Archive Status



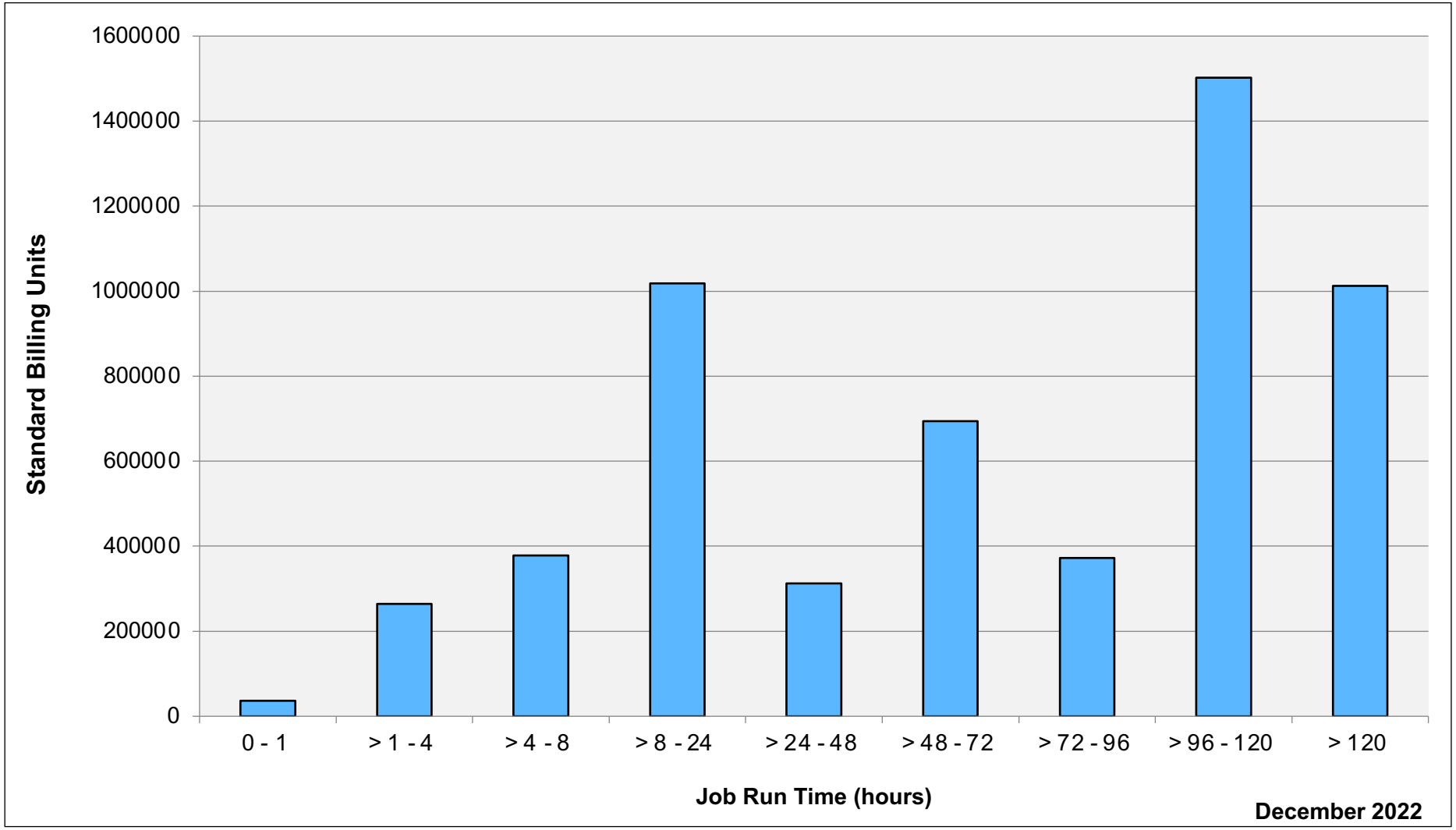
Aitken: SBUs Reported, Normalized to 30-Day Month



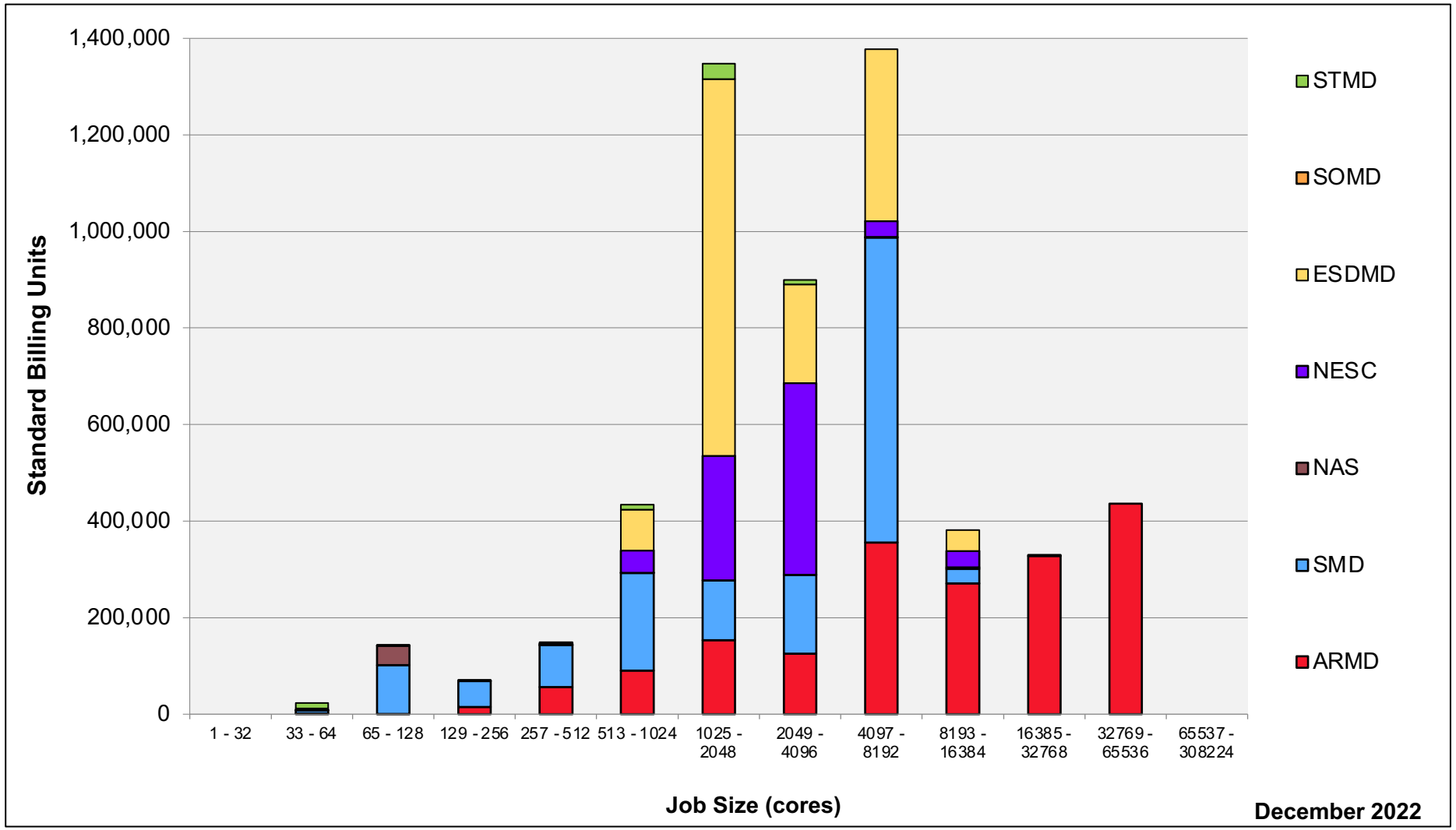
Aitken: Devel Queue Utilization



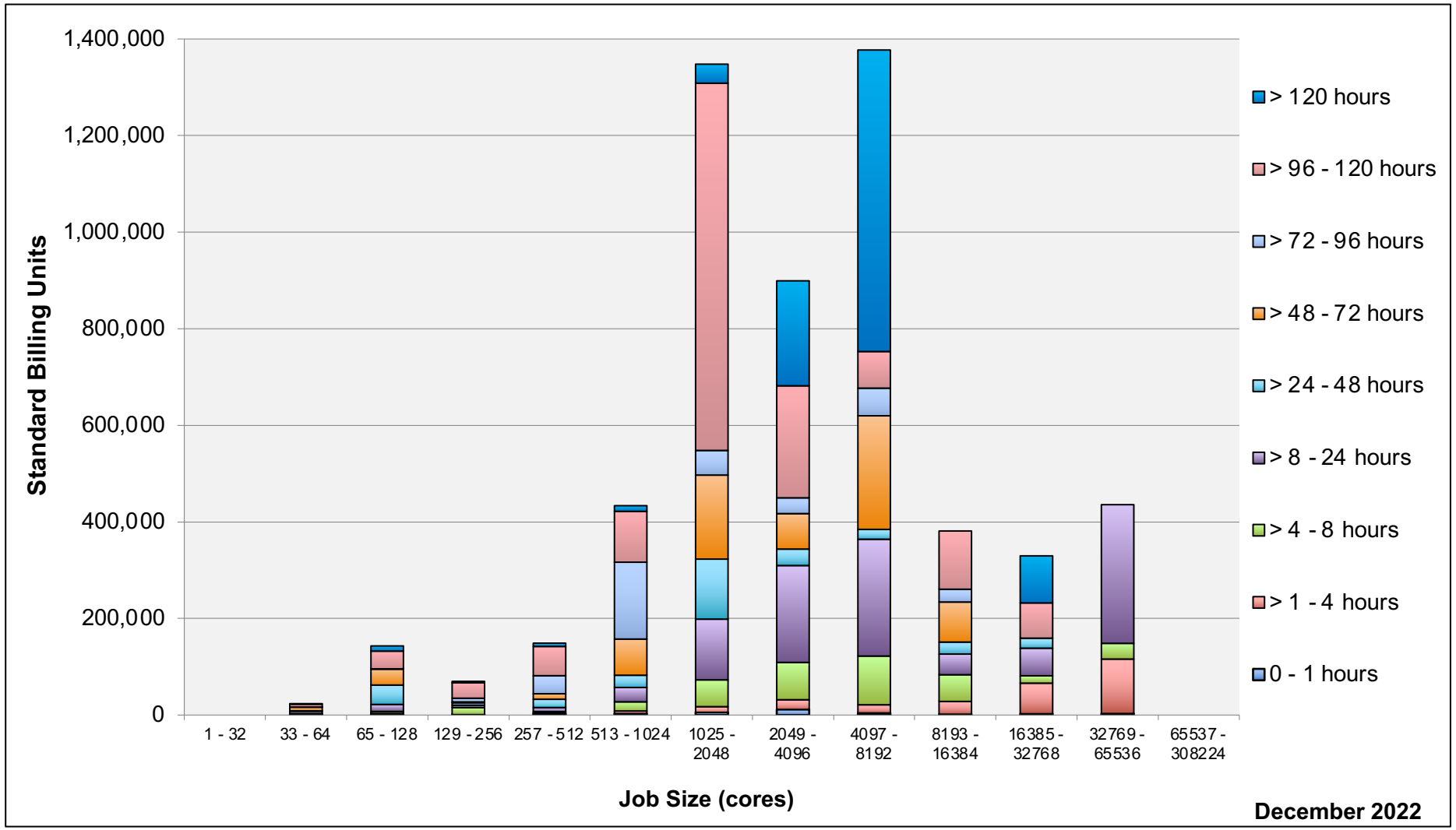
Aitken: Monthly Utilization by Job Length



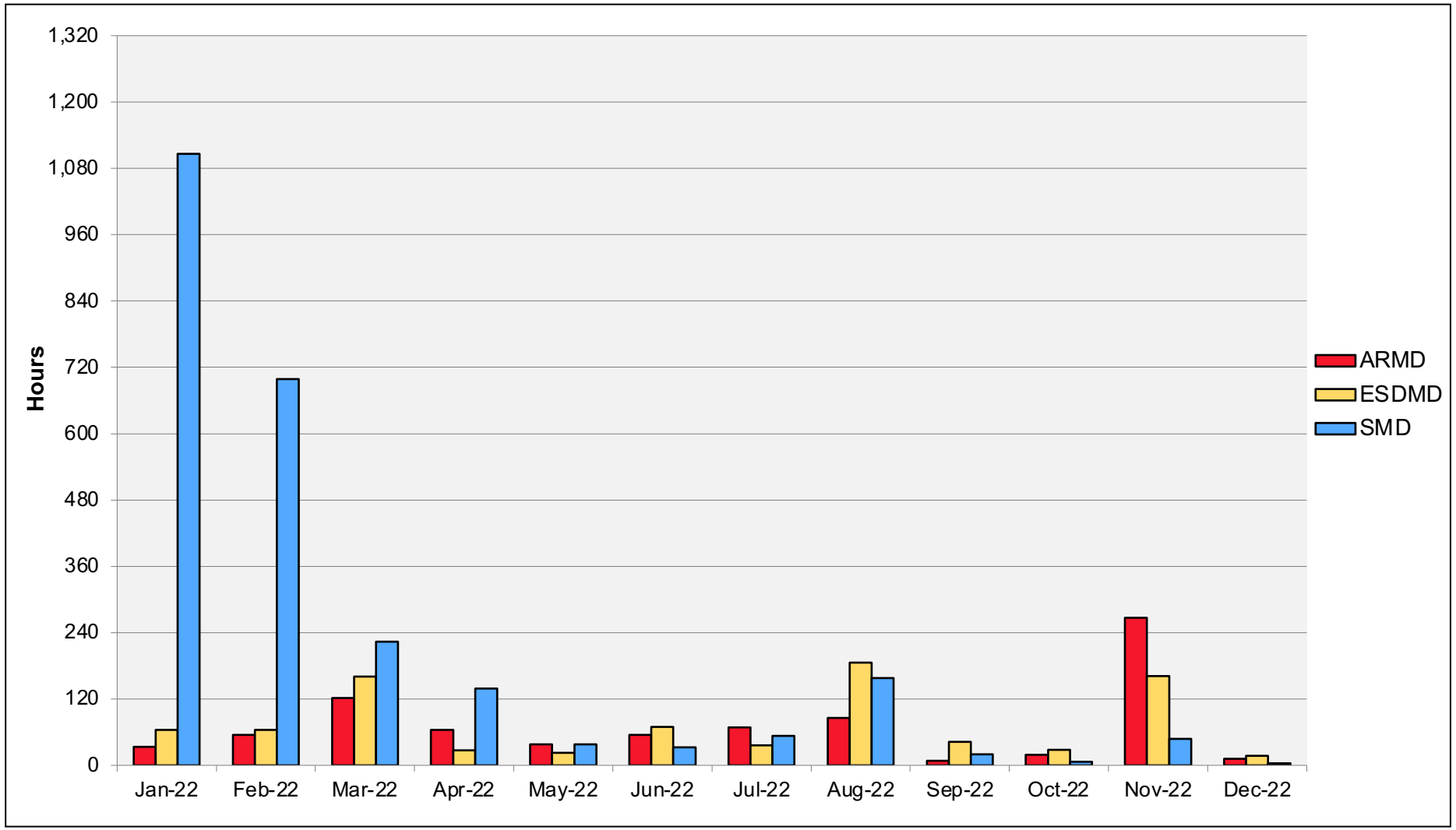
Aitken: Monthly Utilization by Job Size



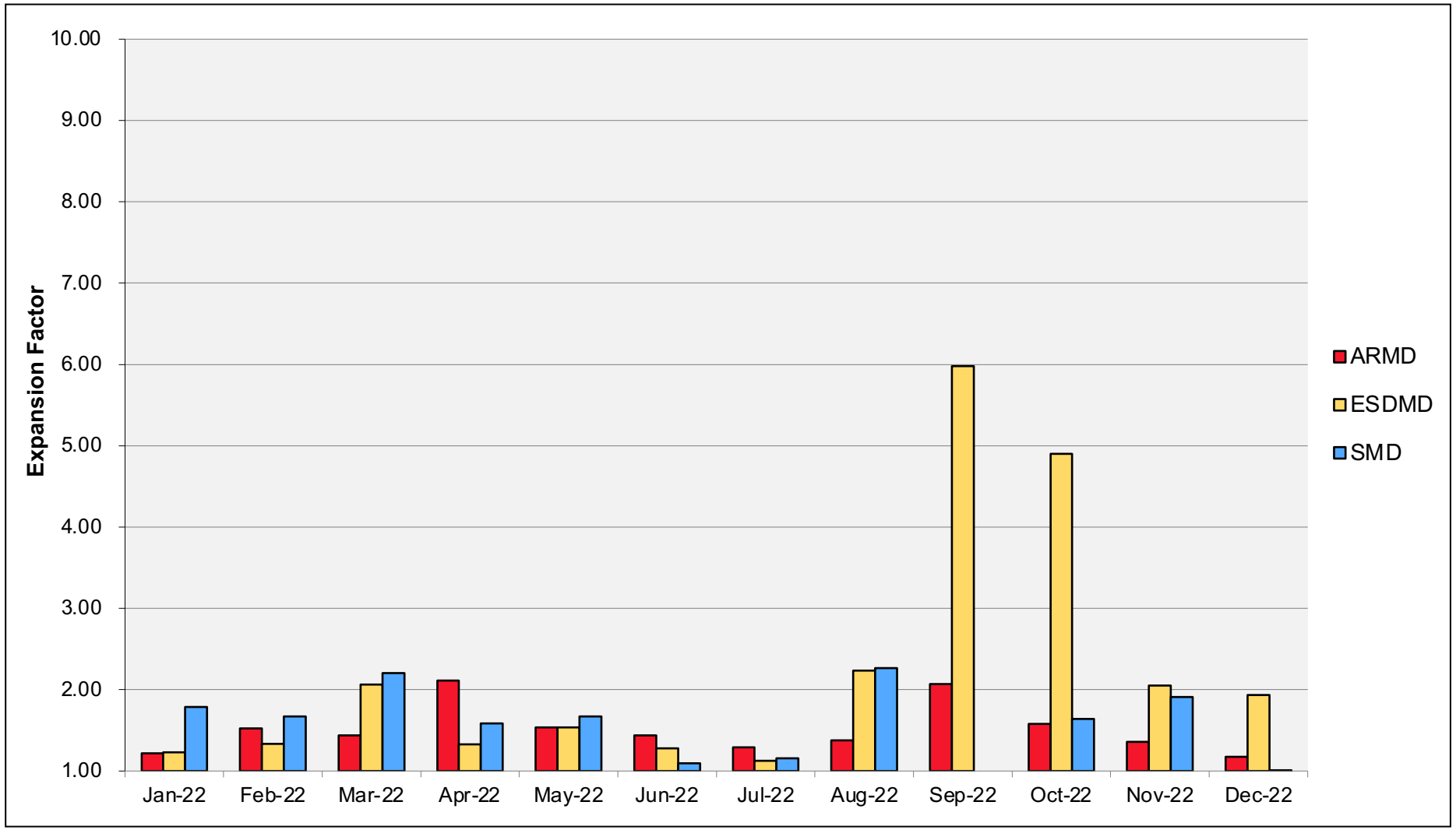
Aitken: Monthly Utilization by Size and Length



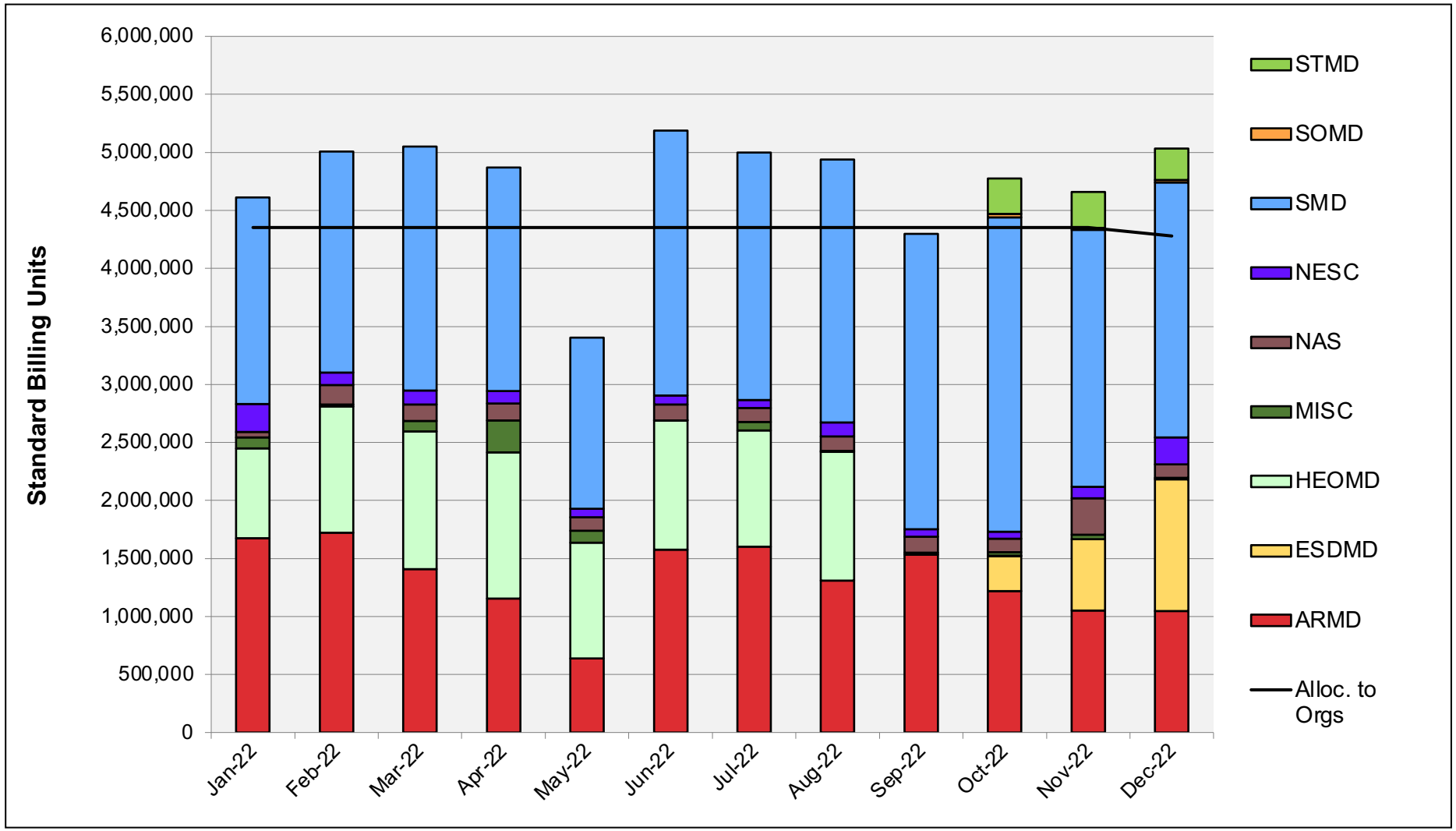
Aitken: Average Time to Clear All Jobs



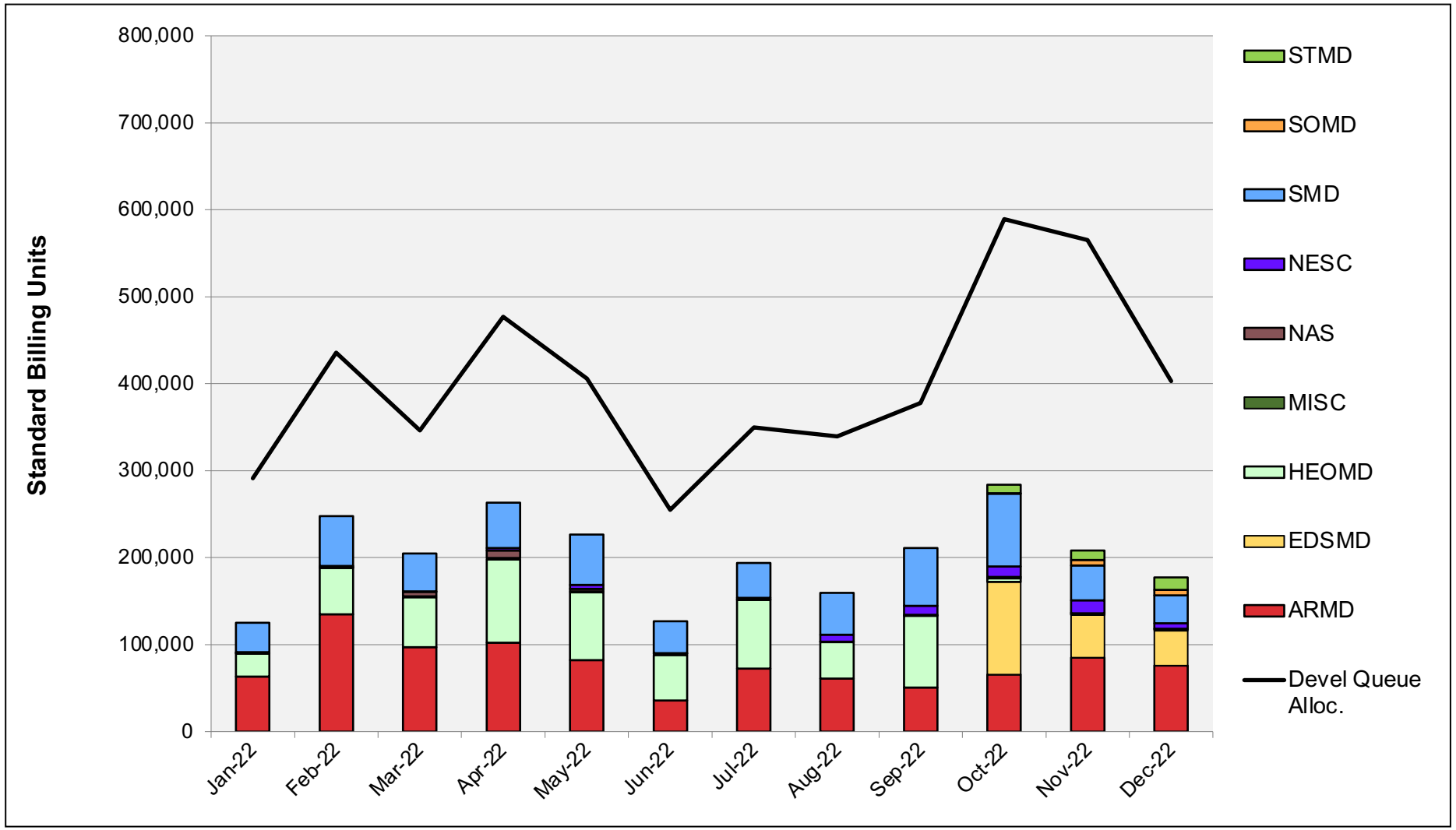
Aitken: Average Expansion Factor



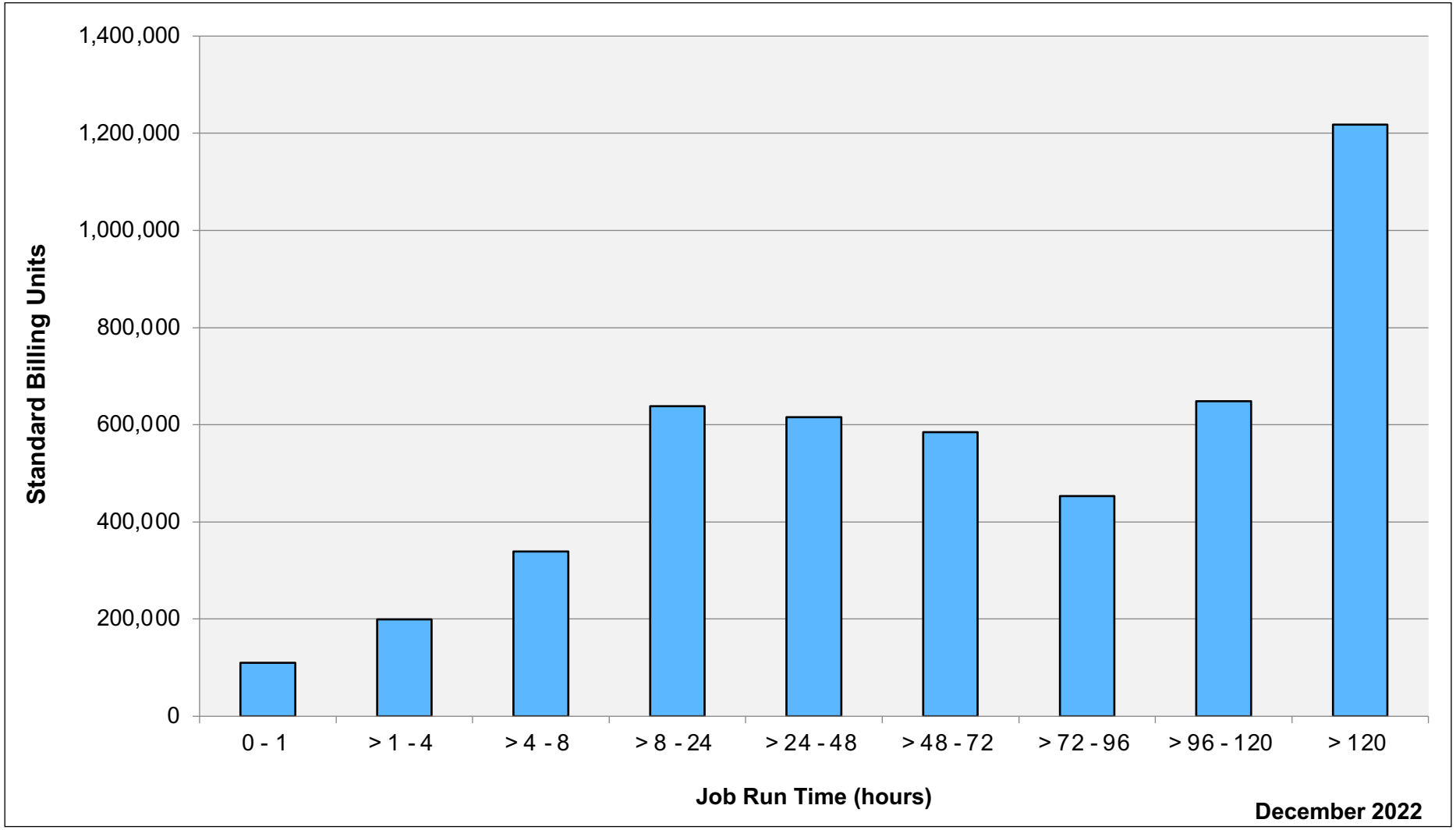
Pleiades: SBUs Reported, Normalized to 30-Day Month



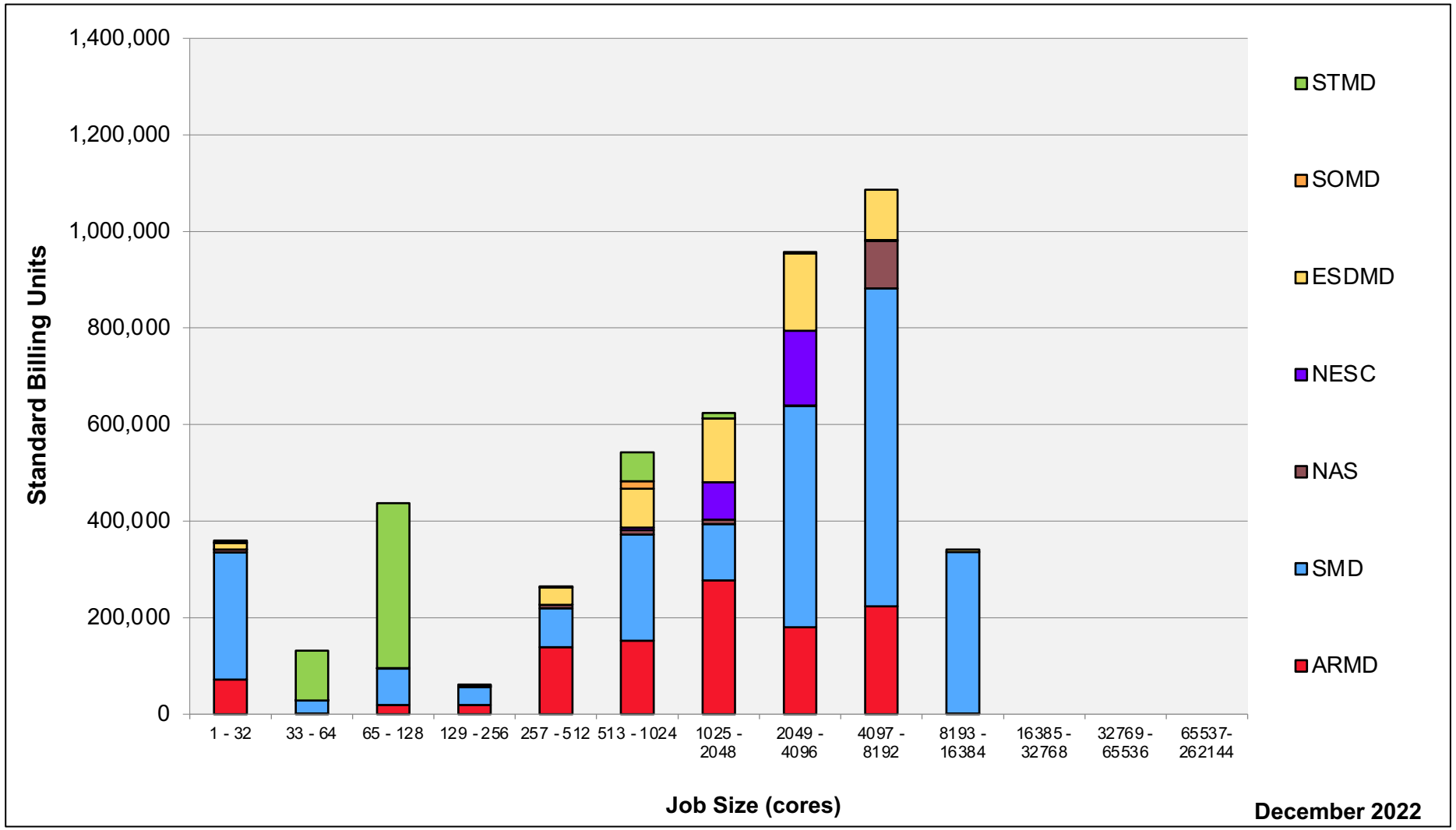
Pleiades: Devel Queue Utilization



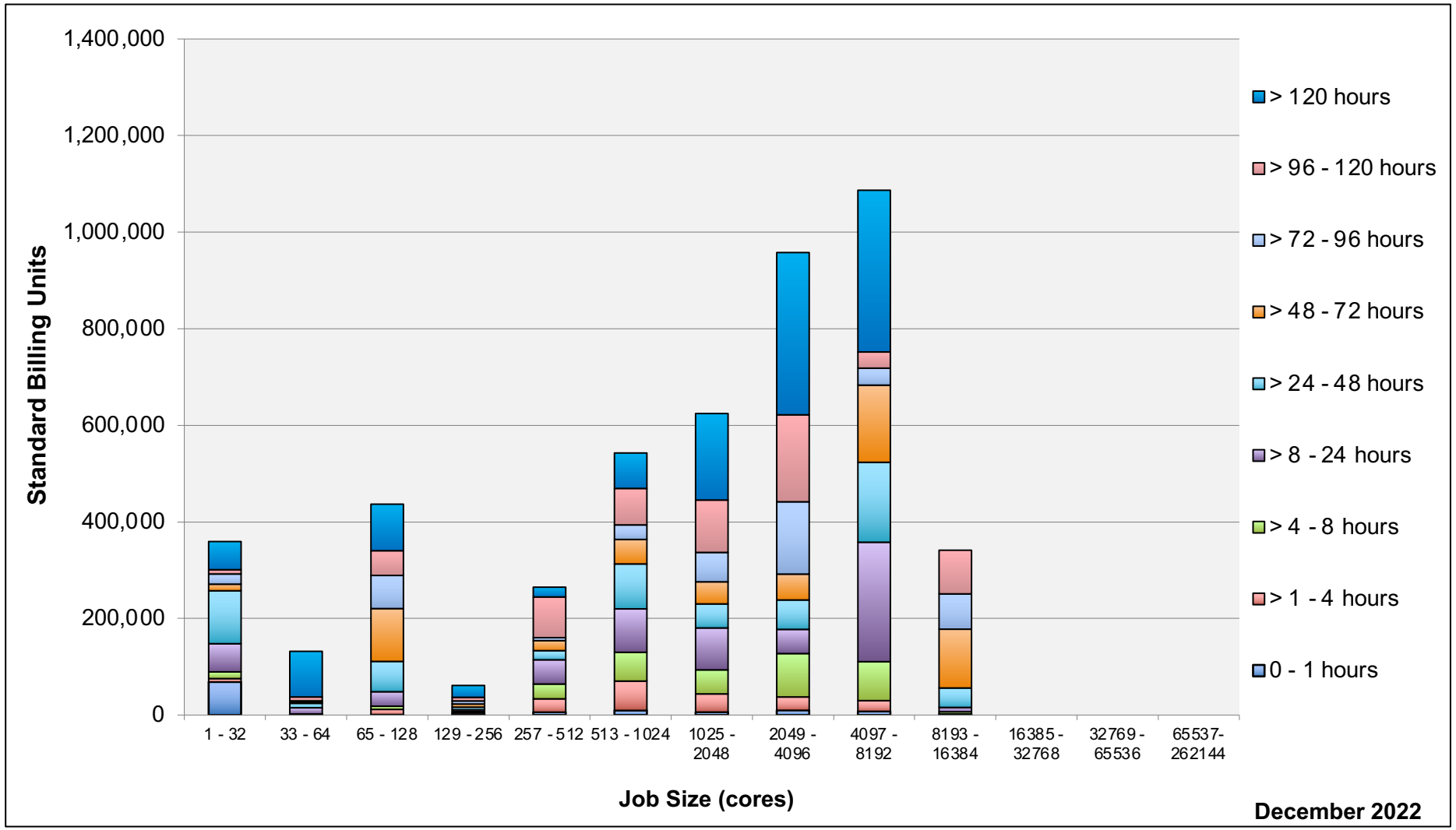
Pleiades: Monthly Utilization by Job Length



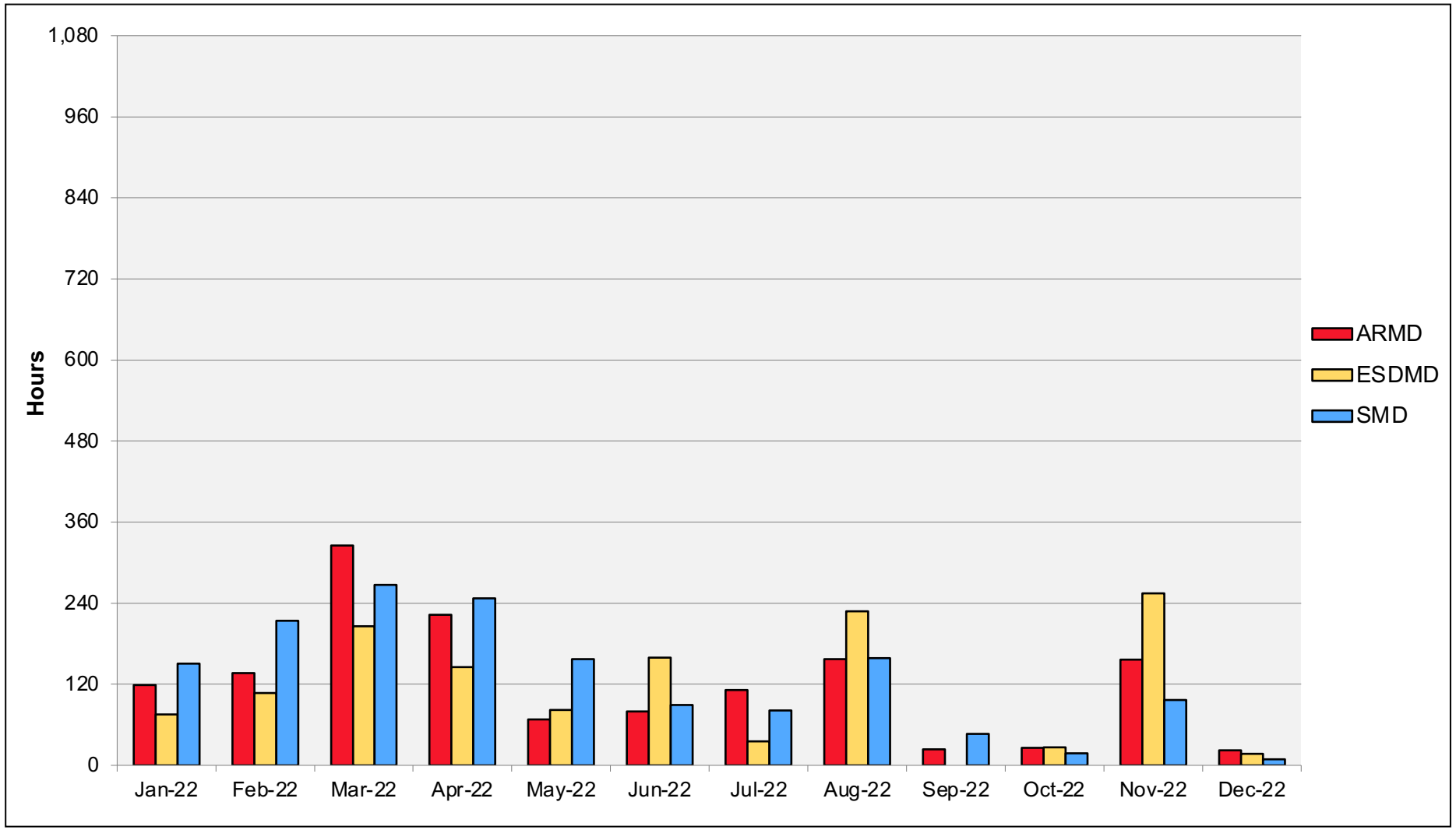
Pleiades: Monthly Utilization by Job Size



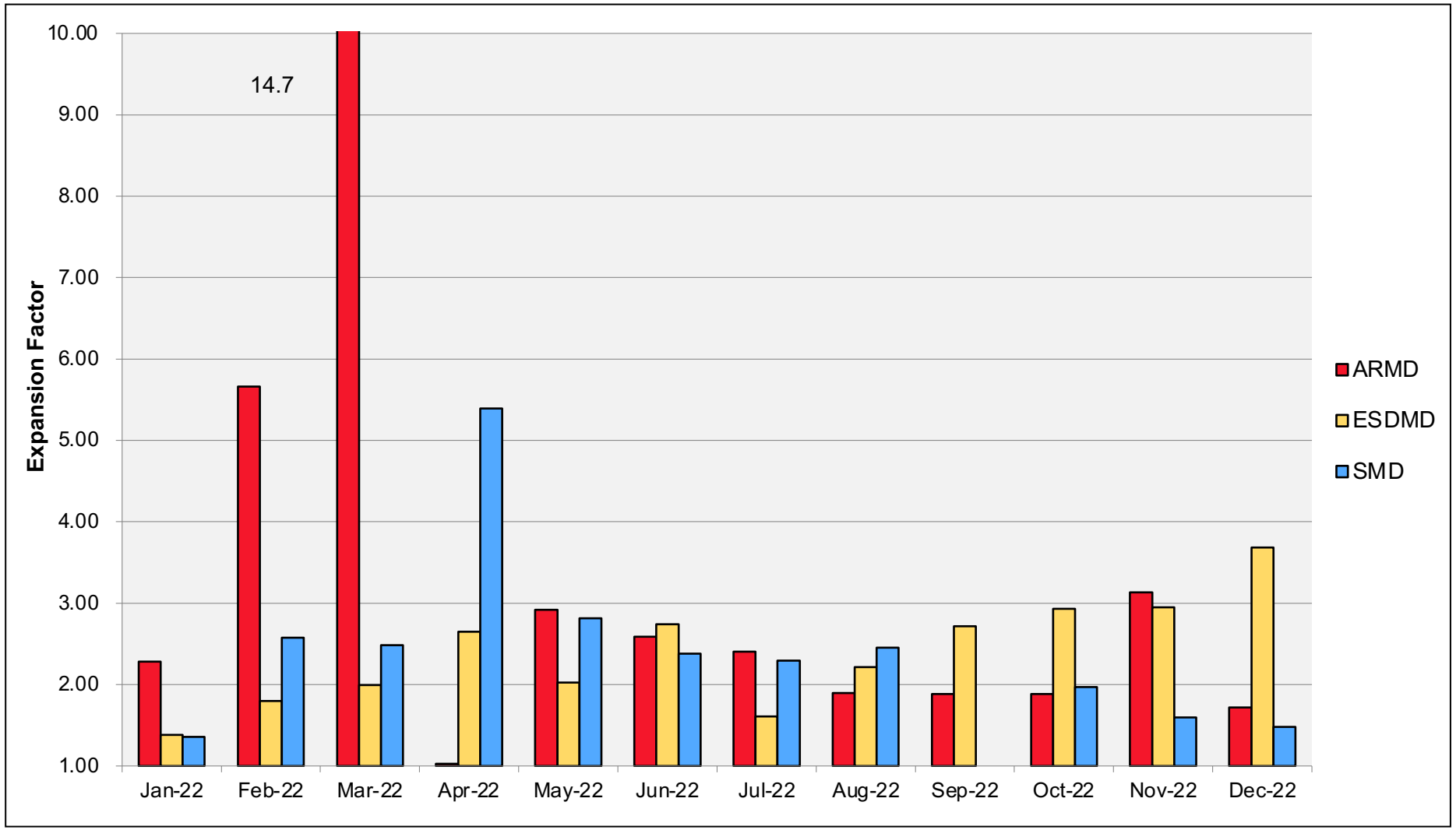
Pleiades: Monthly Utilization by Size and Length



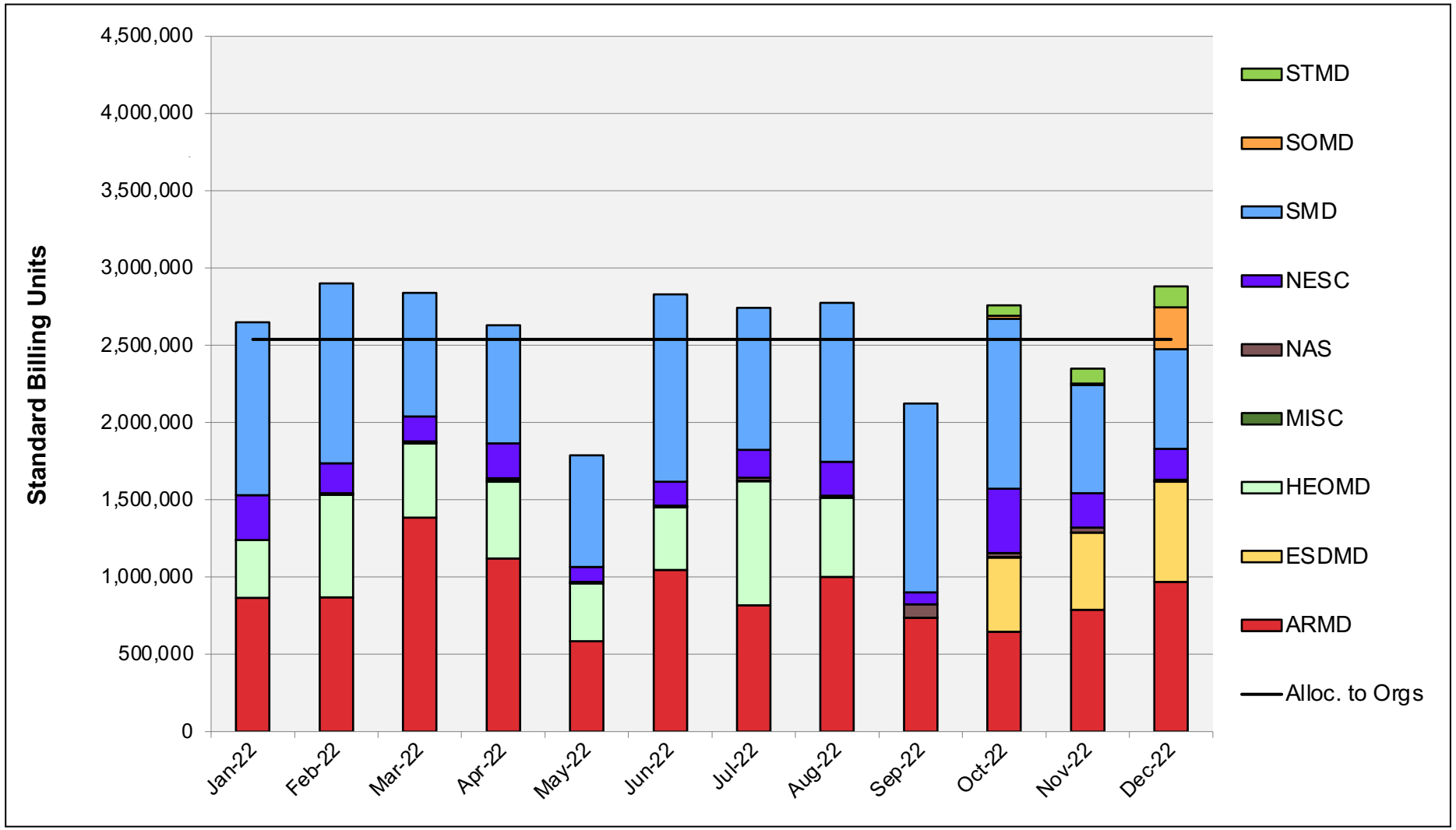
Pleiades: Average Time to Clear All Jobs



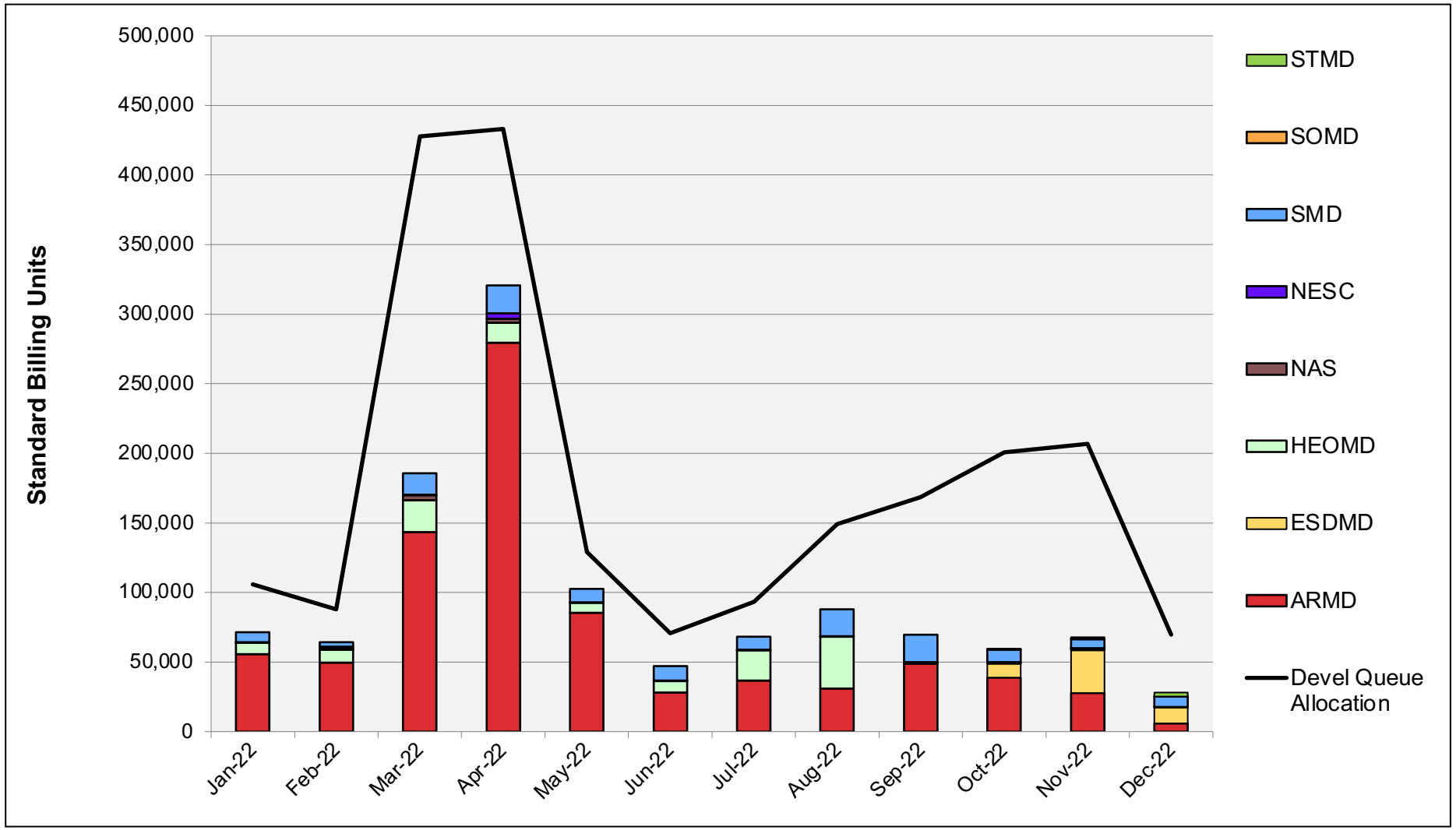
Pleiades: Average Expansion Factor



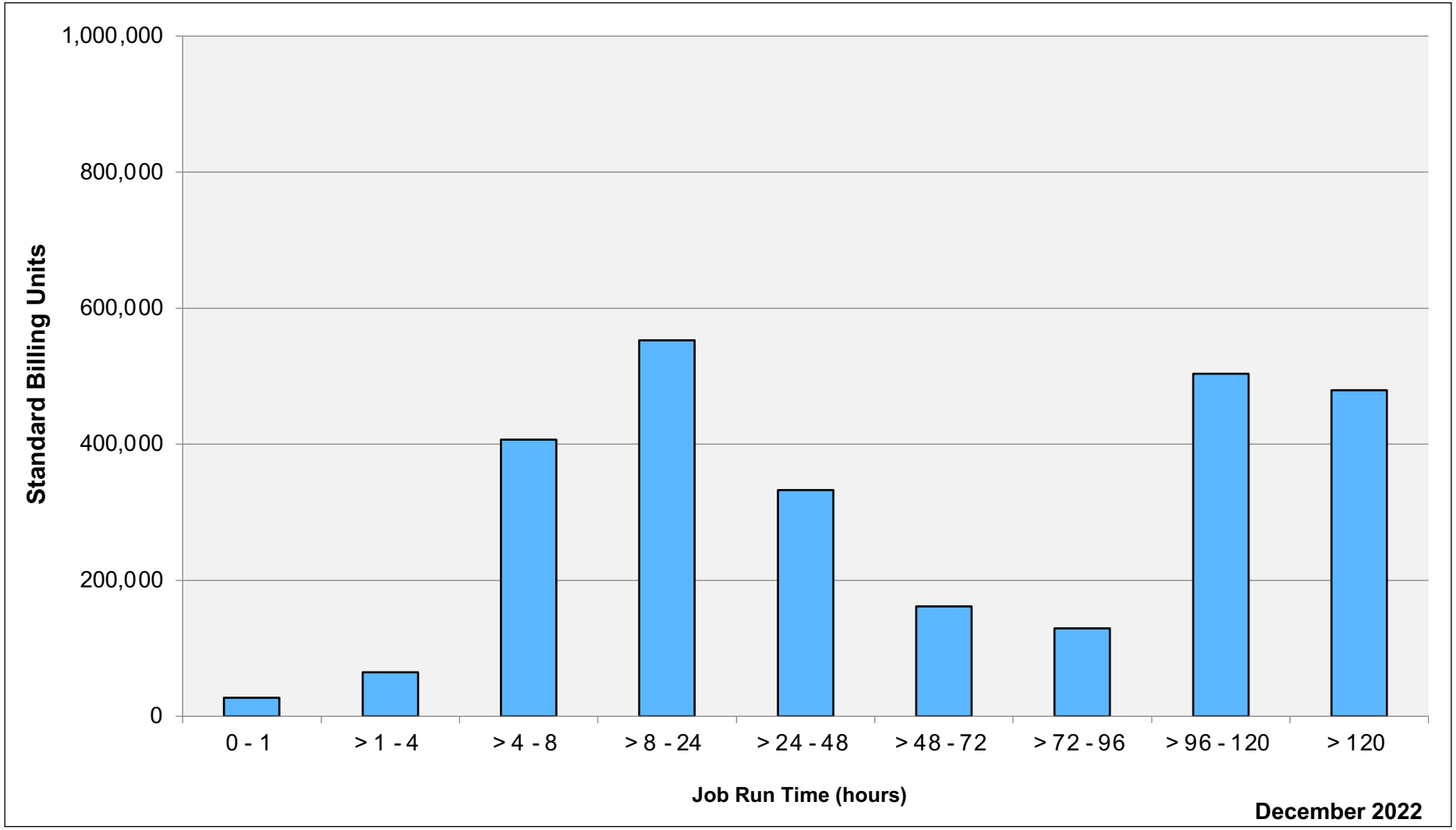
Electra: SBUs Reported, Normalized to 30-Day Month



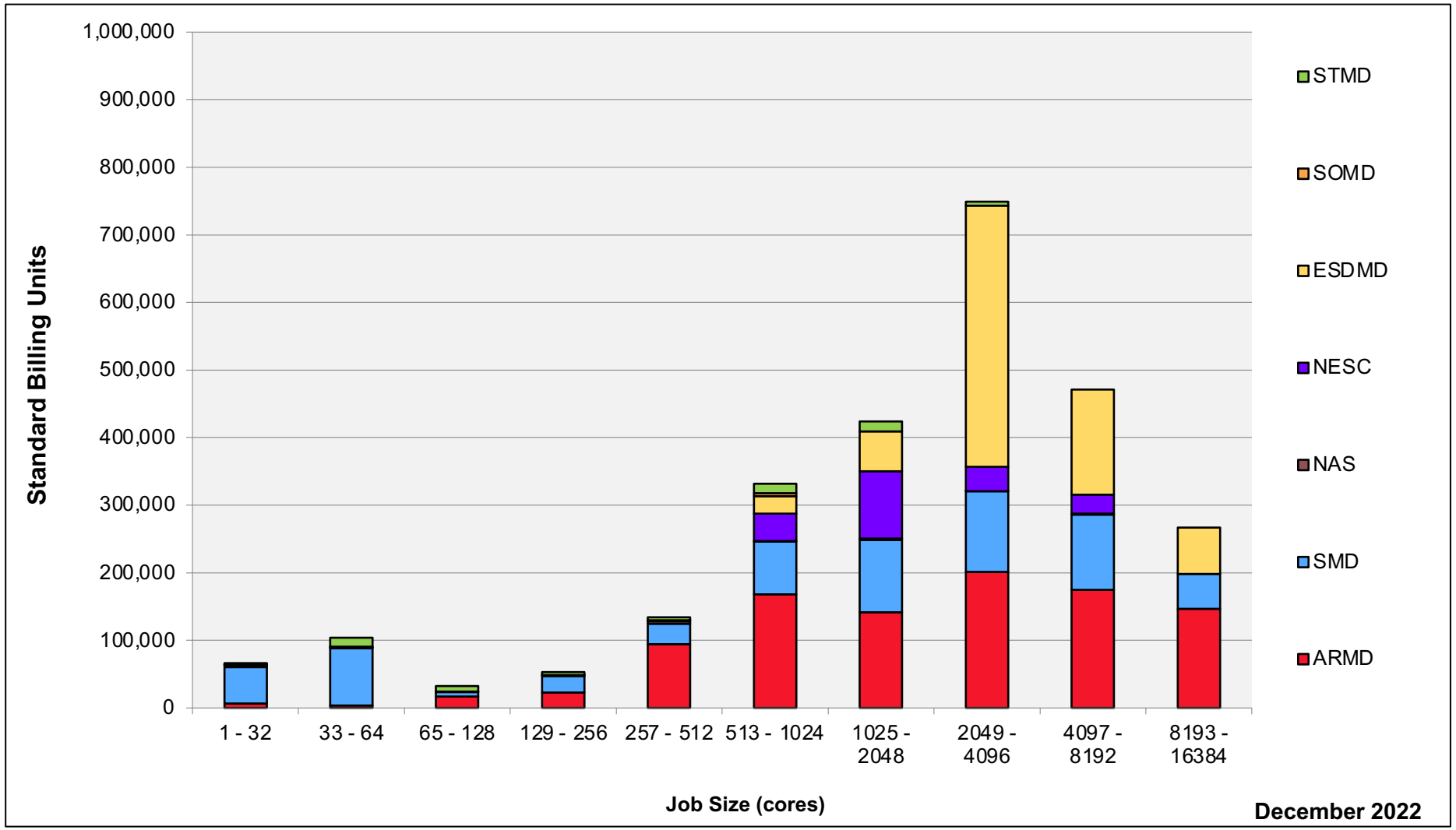
Electra: Devel Queue Utilization



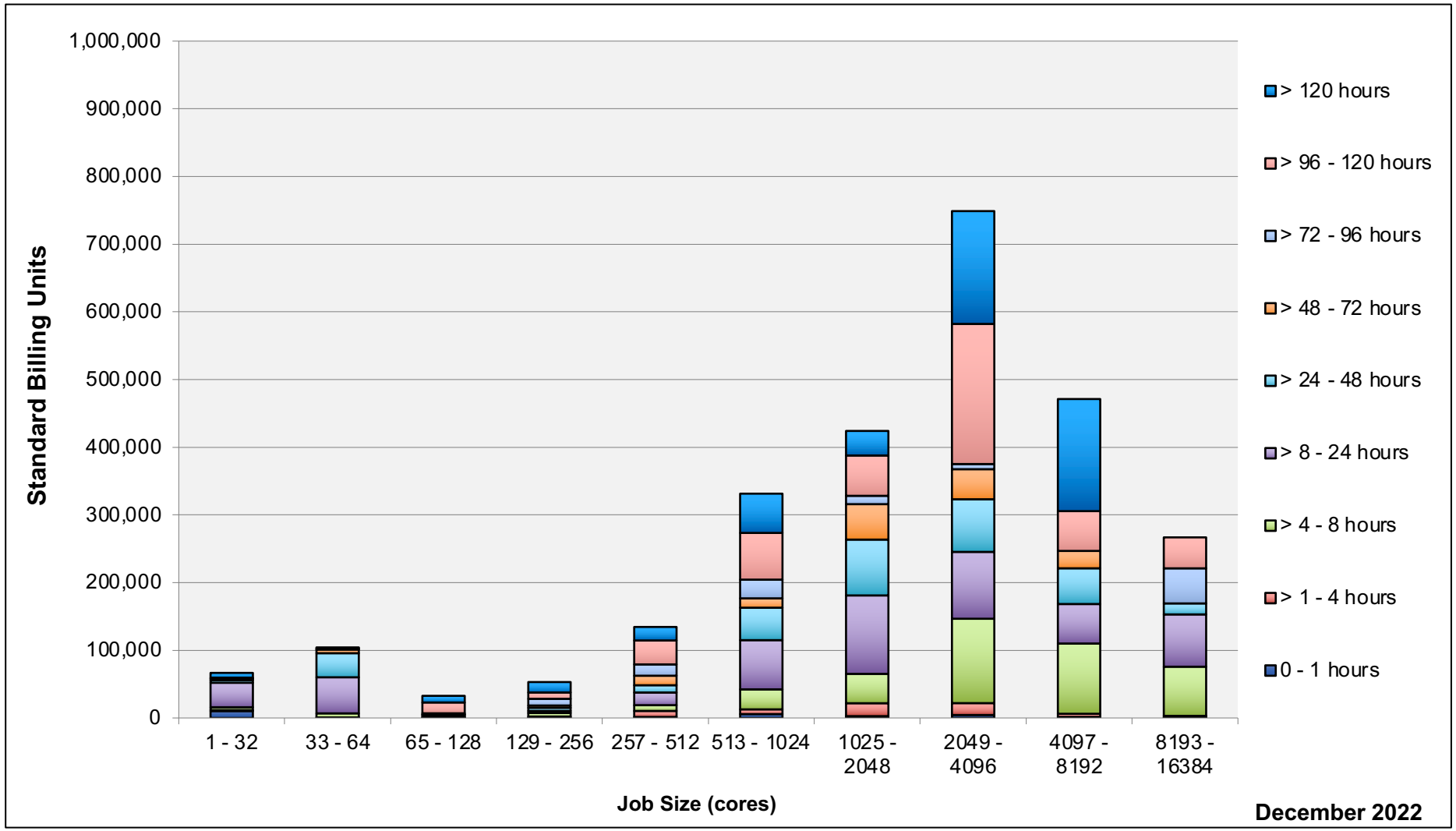
Electra: Monthly Utilization by Job Length



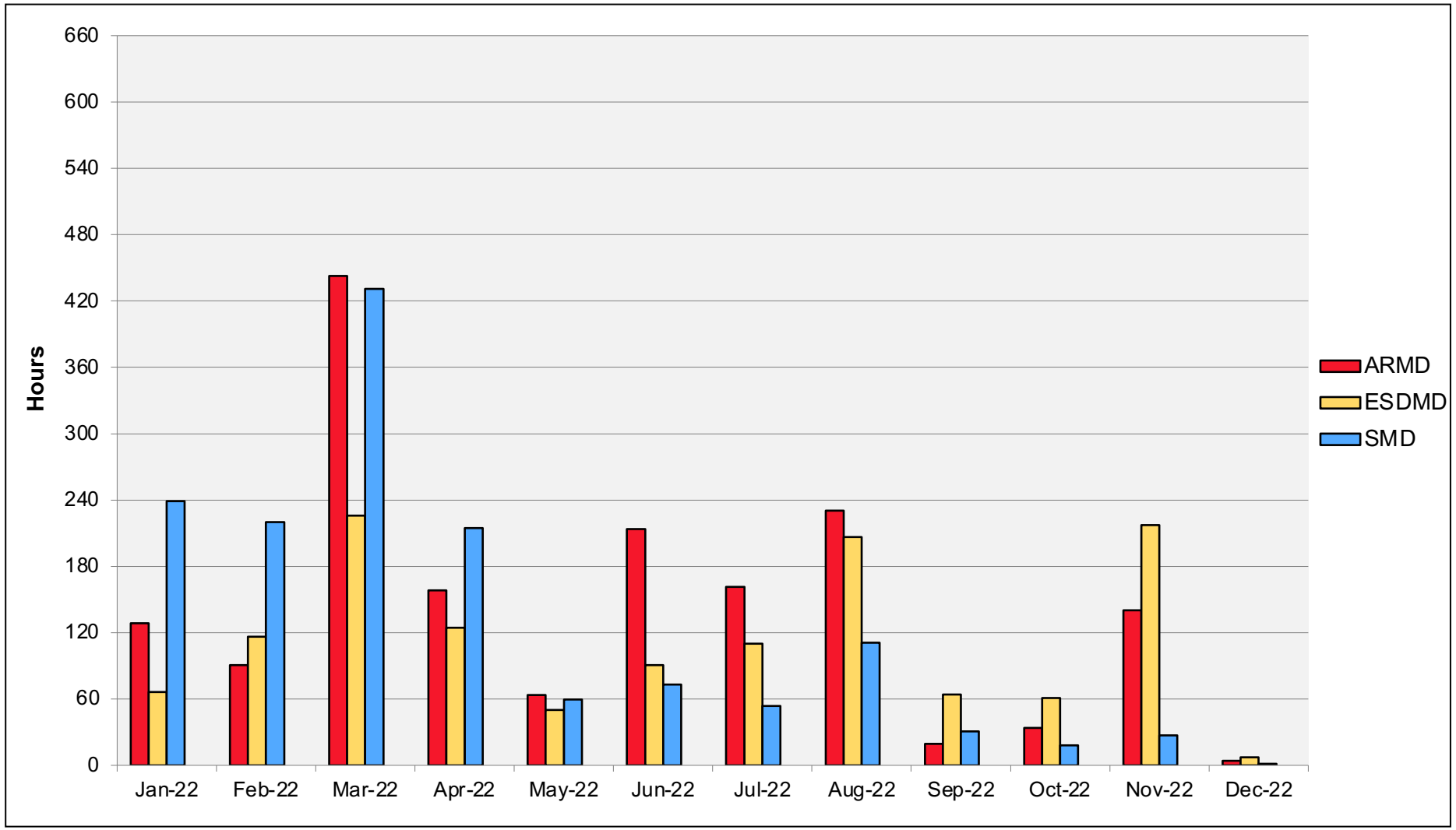
Electra: Monthly Utilization by Job Size



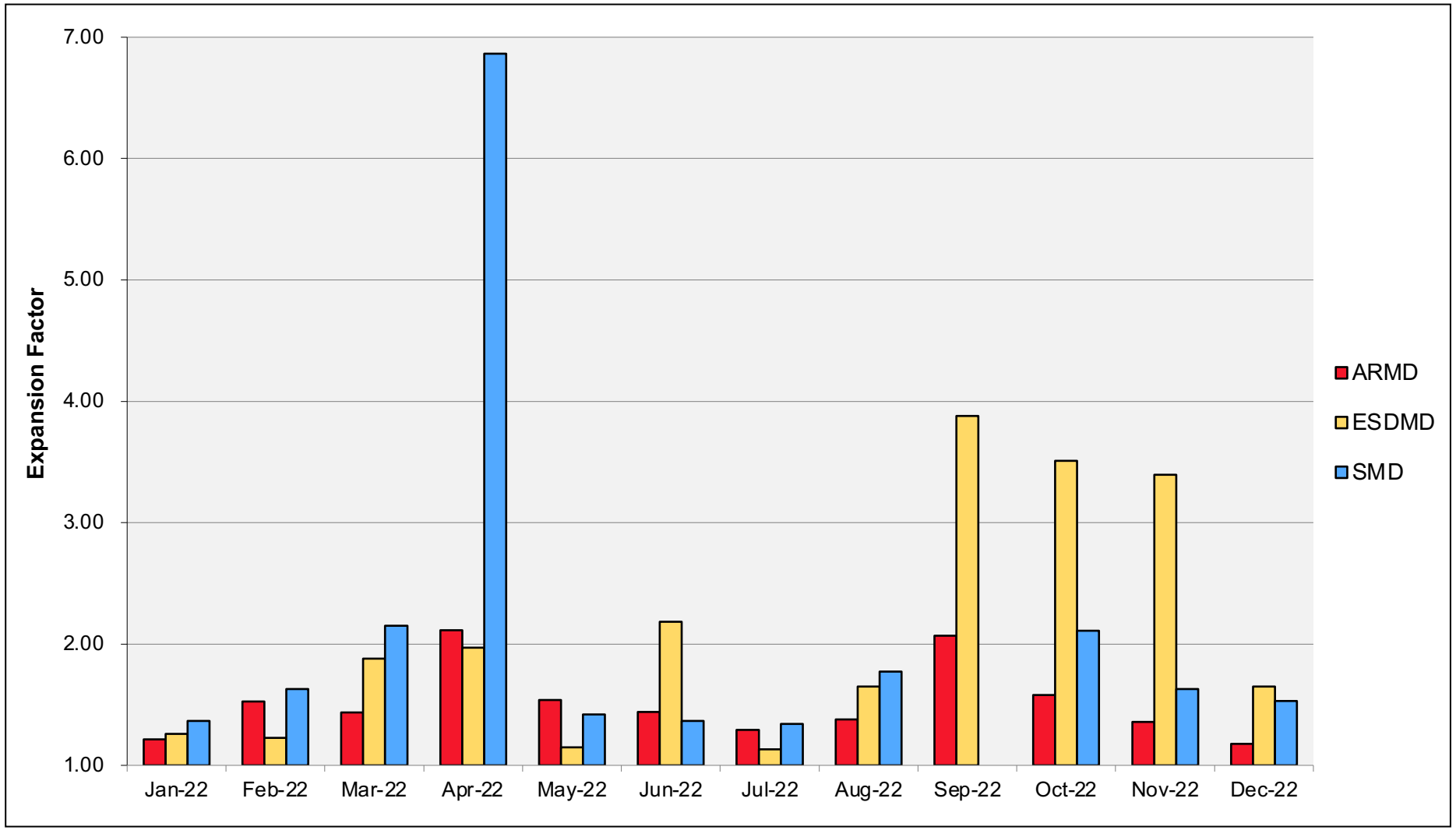
Electra: Monthly Utilization by Size and Length



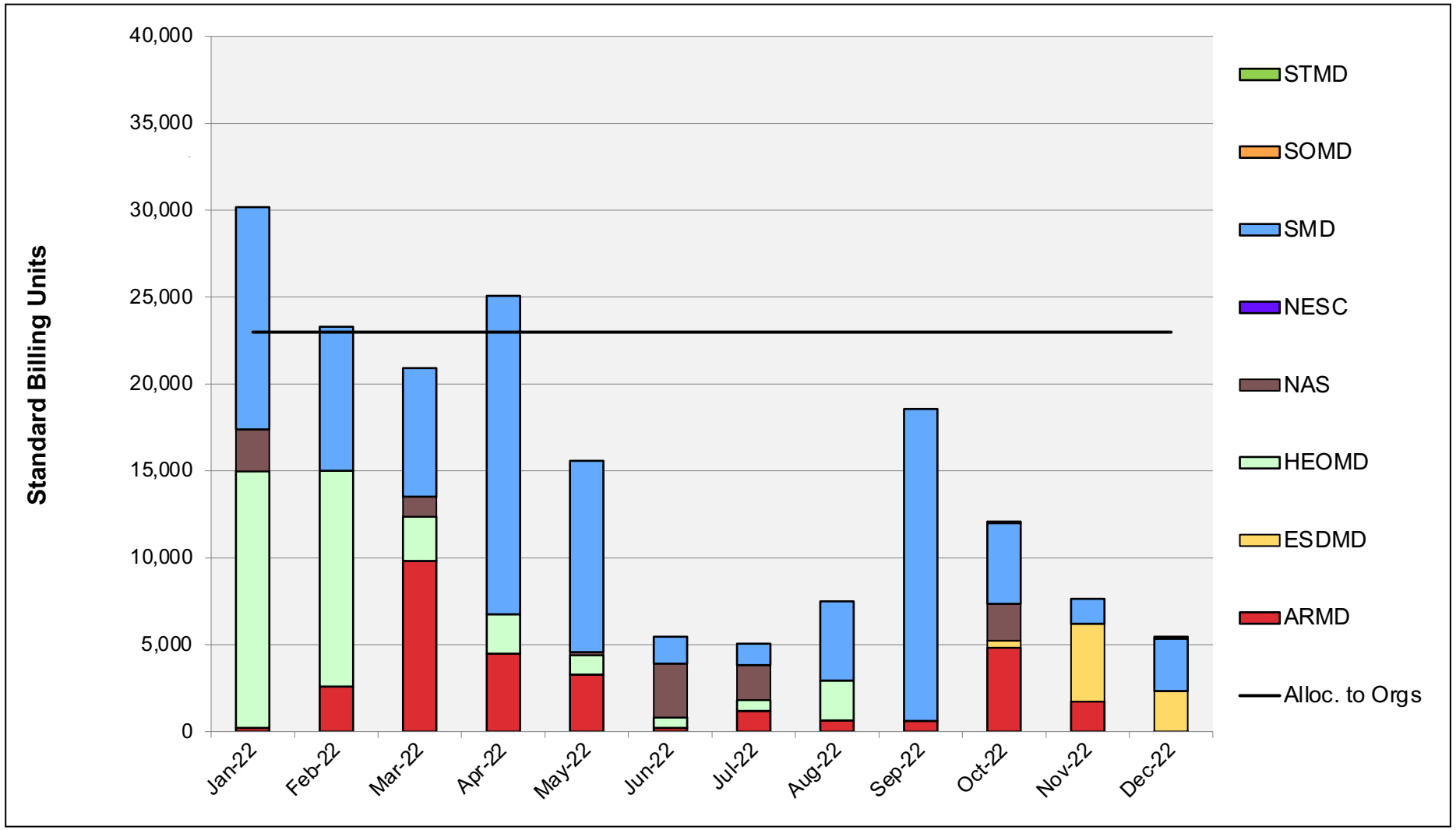
Electra: Average Time to Clear All Jobs



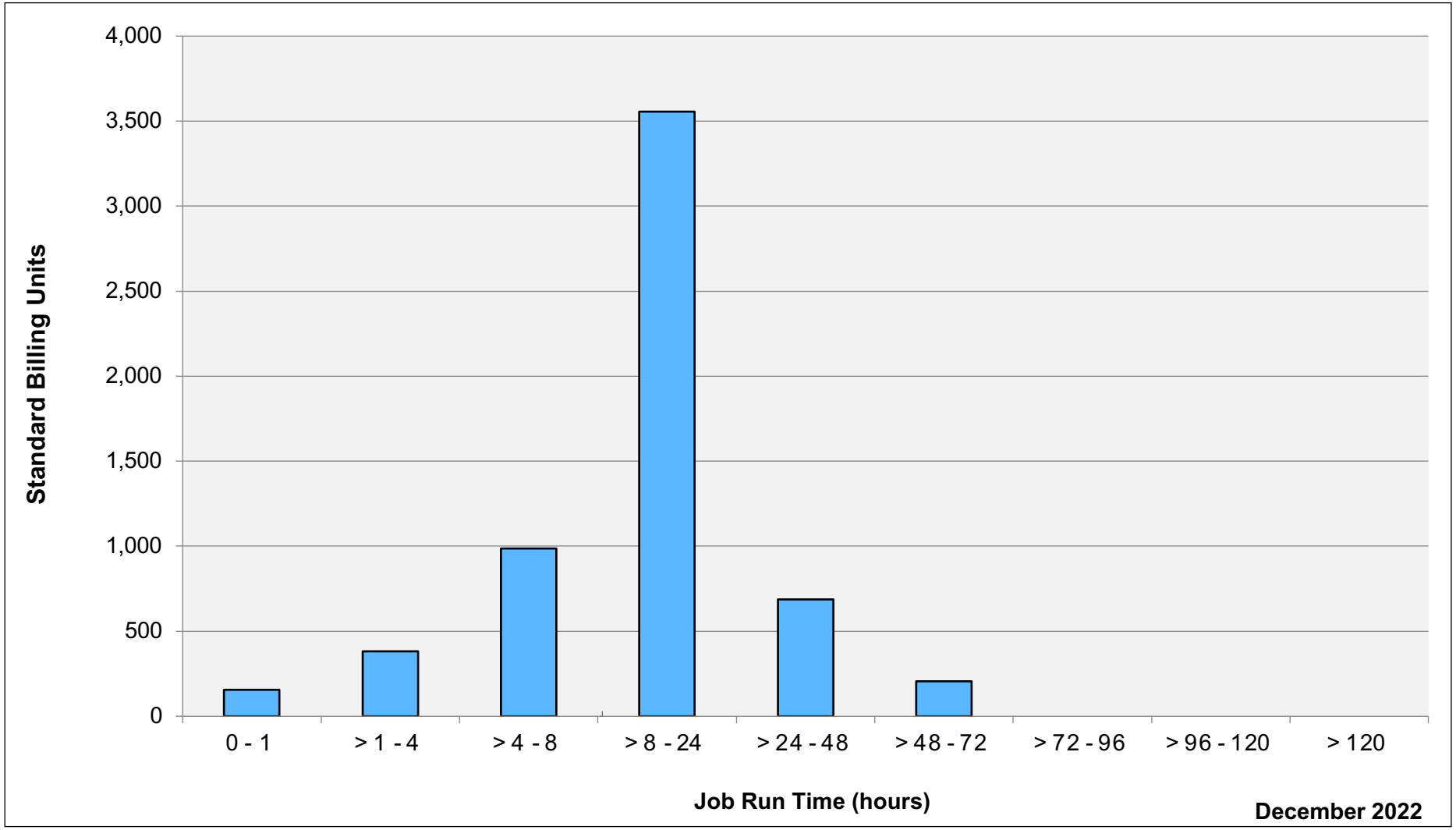
Electra: Average Expansion Factor



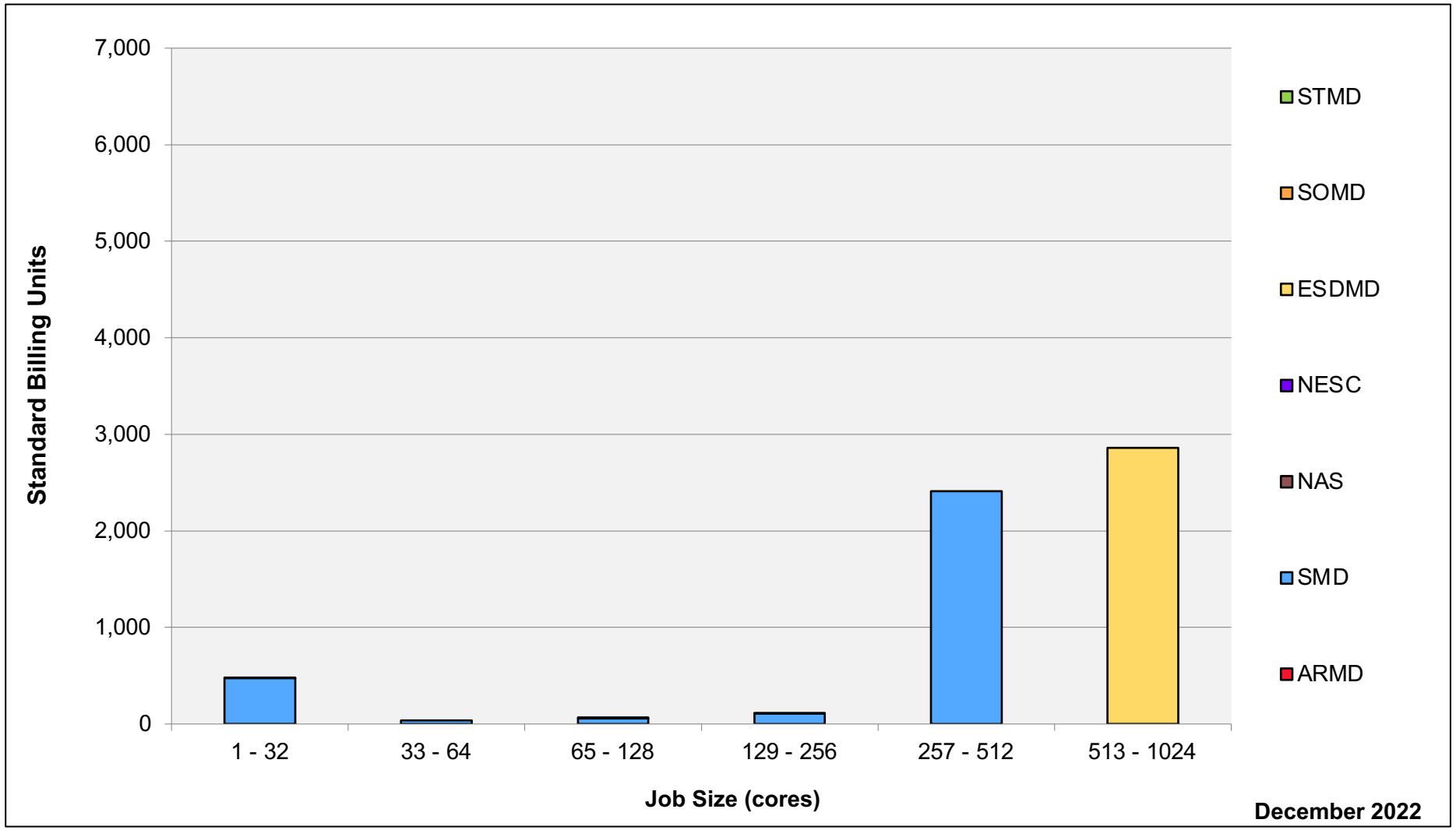
Endeavour: SBUs Reported, Normalized to 30-Day Month



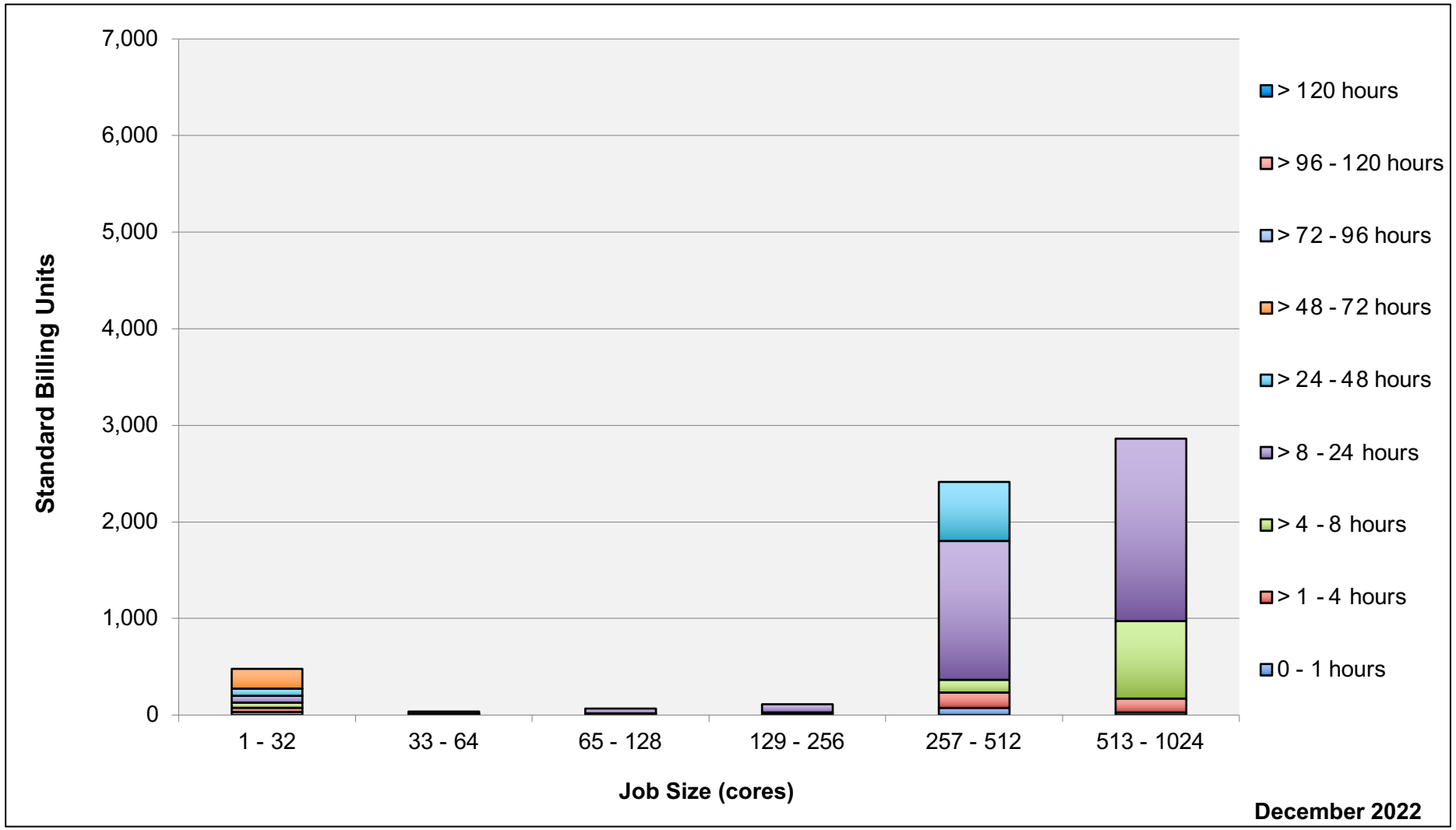
Endeavour: Monthly Utilization by Job Length



Endeavour: Monthly Utilization by Job Size



Endeavour: Monthly Utilization by Size and Length



Endeavour: Average Expansion Factor

